Table 5-7. Summary of U(VI) K_rs calculated for four surface complexation models calibrated to U(VI) breakthrough in column experiments at pH 8.48

[K_r, retardation coefficient; mM, millimoles per liter]

	Quartz	Montmorillonite	Goethite	Ferrihydrite	Ratio $K_r$max:$K_r$min
Site density (mM)	12	7.3	1.1	3.3	
Big Lost River	183	56	6,919	454	124
EBR 1	26	23	46	36	2
USGS 112	75	55	236	143	4
USGS 8	17	14	45	31	3
USGS 19	21	15	110	62	7
USGS 87	51	43	89	67	2
USGS 89	77	72	69	68	1
USGS 90	43	36	80	59	2
NPR test	19	15	62	39	4
P&W 2	43	61	104	70	2
RWMC production	25	22	58	41	3
USGS 92	4	3	8	6	2
Minimum[1]	4	3	8	6	
Median	26	23	69	59	
Average	36	33	82	56	
Maximum	77	72	236	143	
Ratio $K_r$max:$K_r$min	22	21	31	24	

[1]Minimum, median, average, and maximum values exclude the Big Lost River K_r values

5.5.4.2.1 Description of the Np transport simulations

The one-dimensional transport simulations were set up as follows. Water sampled from well USGS 92 (composition given in section 4.3.2), a well in the SDA, screened in a perched-water zone above the C-D interbed, was used as the background water in the one-dimensional column. The water from well USGS 92 is predominantly a $NaHCO_3$-rich water. The 100-m-long one-dimensional column was subdivided into 100 cells, each of which contained 1 kg H_2O (background water) and a goethite surface with $5x10^{-7}$ mol of surface sites per kg of H_2O and a surface area of 54 m^2 per kilogram of H_2O. The composition of the goethite surface at equilibrium with the composition of water from well USGS 92 was calculated by PHREEQC and used as the initial surface composition in the transport simulations. The number of surface sites was decreased by a factor of 10 from the concentration used in section 4.3.2, simply for the convenience of obtaining a retardation factor of about 20 for Np, rather than the factor of about 200 estimated in section 4.3.2. This modification resulted in a decrease by a factor of 10 in the number of timesteps that needed to be considered, thereby reducing by the same factor the time required for the transport simulations. Under these conditions, each one of the Np transport simulations presented here took 50 to 60 hours to run on an Intel Pentium-II personal computer running at 300 MHz.

A dispersivity of 10 m was assumed in the calculations. This dispersivity is probably too high by at least a factor of 10 to reasonably describe transport at the INEEL site but was used to determine whether constant retardation of Np transport still could be obtained in such a system. Simulations with lower dispersivity, or simulations with a dispersivity of 0 m, would have required significantly less (10 times less) computer time to run.

Water from well USGS 112 (composition given in section 4.3.2), a $CaHCO_3$-rich water modified to include 10^{-8} mol Np and 10^{-8} mol Pu, was used to simulate the infiltration of contaminated water into the column.[3] The average linear ground-water velocity simulated was 10 m/yr. The infiltration of Np- and Pu-contaminated water lasted for 2,500 timesteps (250 years). After 2,500 timesteps, the aqueous solutions in the column had a uniform concentration of 10^{-8} mol Np and Pu, and the goethite surfaces were in equilibrium with these Np and Pu concentrations throughout the entire column. At that point, background water from well USGS 92 (containing no Np or Pu) was allowed to infiltrate into the column for up to 6,000 timesteps (600 years), thereby simulating the cleanup of the column.

Water from both well USGS 92 and well USGS 112 was slightly supersaturated with respect to calcite and with respect to chalcedony. In some, but not all, simulations, these minerals were not specified as initially present in the column but were allowed to precipitate to allow the water to reach equilibrium. Any calcite precipitated was allowed to redissolve later on in the simulation if necessary.

Np and Pu thermodynamic data were added to the default PHREEQC data base from two different sources (discussion in section 4.3.2): (1) the ANSTO thermodynamic data base (provided by Marianne Guerin, 1998; Np and Pu data in that data base are identical to those contained in the HATCHES data base, Cross and Ewart, 1991), and (2) the EQ3/6 data base (provided by David Turner, Southwest Research Institute, written commun., 1999). Np and Pu surface complexation data compiled by Turner (1995) were added to both data bases. For the purposes of this report, the data bases created from the ANSTO and EQ3/6 data bases will be referred to as the "ANSTO" and "EQ3/6" data bases, even though these are not the complete ANSTO and EQ3/6 data bases.

5.5.4.2.2 Np infiltration results

Results obtained for the Np infiltration phase of the simulations (figs. 5-17 and 5-18) show that Np breakthrough at the end of the column occurred after approximately 17 pore volumes (1,700 time steps). Speciation calculations in section 4.3.2 predicted a retardation of about 20 given the sorption site concentration used in the transport simulations. The retardation of Np transport appears relatively constant in the figures, which indicates that the retardation could have been predicted using a constant K_d approach instead of the surface complexation approach. However, an appropriate K_d might have been difficult to predict.

Transport of Np was about 10 percent faster in the simulations that allowed calcite precipitation (and later redissolution) than in those that didn't allow calcite precipitation. Allowing calcite precipitation resulted in a decrease in pH of the infiltrating solution from a value of 8.4 (before calcite precipitation) to values below 7.9. This resulted in a decrease in the number of neutral and negatively charged sorption sites and, therefore, resulted in a decrease in the amount of sorbed Np (section 4.3.2.3, table 4-6, for the predominant Np surface complexes on goethite).

During the Np infiltration phase, Np transport was approximately 10 percent faster in the simulations con-

[3] 10^{-8} M of ^{237}Np corresponds to approximately 62 Bq/kg H_2O or 1,670 pCi/kg H_2O.

ducted with the ANSTO data base than in those conducted with the EQ3/6 data base (figs. 5-17 and 5-18). As discussed in section 4.3.2.2, the ANSTO data base predicts that significant amounts (about 15 percent) of Np(VI) will be present in the water from well USGS 112, whereas the EQ3/6 data base predicts that essentially all the Np will be in the Np(V) state. The databases do not contain any data for Np(VI) surface complexes, only for Np(V) complexes; therefore, any aqueous Np(VI) species present become unavailable for sorptive retardation during transport.

Breakthrough curves (fig. 5-19) constructed from the results of the Np infiltration simulations for a point at the end of the 100-m-long column, using either the ANSTO or EQ3/6 data bases with or without specification of calcite equilibrium, are relatively similar to the curves that would be obtained for simulations of reactive transport with a constant K_d approach, with one significant exception. The curves for the PHREEQC simulations show an abnormally steep leading edge (the left portion of each curve), compared with the curve that would be obtained from a simulation that used a constant K_d approach. The most likely reason for this behavior is that Np exhibits relatively stronger sorption at small aqueous concentrations than at large aqueous concentrations. In other words, the effective K_d that may be applied to the PHREEQC simulation results is not constant and, instead, decreases with increasing aqueous Np concentrations (see discussion at the end of this section). The breakthrough curves for the PHREEQC simulations also clearly illustrate (1) the greater Np retardation in the simulations conducted with the EQ3/6 thermodynamic data base than with of the ANSTO data base, and (2) the greater Np retardation in the simulations conducted without specification of calcite equilibrium than in those conducted with calcite equilibrium.

5.5.4.2.3 Np cleanup results

The results of the Np cleanup phase of the simulations show surprisingly greater complexity than do the results of the Np infiltration phase (figs. 5-20, 5-21, 5-22, 5-23). The results of the simulation conducted using the ANSTO data base without specification of calcite equilibrium (fig. 5-20) show that aqueous Np concentrations decrease by about 60 percent throughout the column after flushing of one pore volume (100 timesteps) of initially Np-free water from well USGS 92. However, after flushing by this first pore volume, the rate of cleanup slows down considerably. After flushing by 25 pore volumes, aqueous Np concentrations are still near 10^{-9} mol in the center of the column, or 10 percent of the initial Np-saturated condition; another 25 pore volumes (50 total) are required to halve the aqueous Np concentrations to the $0.5x10^{-9}$ mol level. The results of the simulation conducted using the EQ3/6 data base without specification of calcite equilibrium (fig. 5-21) show similar results to those conducted using the ANSTO data base, except that Np concentrations are reduced even more, by about 90 percent, after flushing by the first pore volume. Np concentrations after flushing with about 50 pore volumes remain at about $0.3x10^{-9}$ mol in the center of the column.

The simulations conducted with specification of calcite equilibrium (with either the ANSTO or EQ3/6 data bases) show faster and more even removal of the sorbed Np and faster cleanup of the contaminated column relative to the simulations conducted without specification of calcite equilibrium. This faster and more evenly distributed removal of Np is the result of the lower sorption capacity of the column for Np at lower pH values. In the results from the simulation conducted with the ANSTO data base (fig. 5-22), aqueous Np concentrations in the first 80 shifts of the cleanup phase rise as much as 5 percent above the maximum aqueous Np concentrations recorded during the Np infiltration phase. In contrast, results from the simulation conducted with the EQ3/6 data base (fig. 5-23) show only a very slight increase in aqueous Np concentrations above the 10^{-8} mol level.

The shape of breakthrough curves (fig. 5-24) constructed from the results of the Np cleanup simulations (ANSTO data base), with or without specification of calcite equilibrium, are significantly different from the shape of "normal" breakthrough curves obtained from simulations of reactive transport with a constant K_d approach. Normal breakthrough curves have, at most, one inflection point. Breakthrough curves for the PHREEQC simulations presented here show three inflection points for the simulations without specification of calcite equilibrium, and four inflection points for the simulations with specification of calcite equilibrium. In the simulations without specification of calcite equilibrium, the relatively fast initial decrease in Np aqueous concentrations, followed by the slight increase and the relatively slow subsequent decrease (caused by the larger effective K_d at small Np concentrations) could not have been modeled by using a constant K_d approach. Similarly, in the simulations with specification of calcite equilibrium, the increase in Np aqueous concentrations above the initial value of 10^{-8} mol also could not have been modeled with a constant K_d approach.

5.5.4.2.4 Np sorption isotherms for the PHREEQC surface complexation models

Np sorption isotherms were calculated on the basis of SCMs used in the PHREEQC speciation and transport simulations discussed in the previous section and in section 4.3.2. Two different types of simulations were conducted (figs. 5-25 and 5-26). In the first type, entitled "$NpCl_5$ addition", as much as 10^{-6} mol of $NpCl_5$ and of $PuCl_5$ were added in 1,000 increments of 10^{-9} mol to a system consisting of 1 L of water from well USGS 112, and a goethite surface with $5x10^{-7}$ mol of sorption sites preequilibrated with water from well USGS 92. In the second type of simulation, entitled "mixture of water," water from well USGS 92 and water from well USGS 112, to which $2x10^{-7}$ mol of Np and Pu had been previously added, were mixed together in various fractions and equilibrated with the goethite surface (that contained $5x10^{-7}$ mol of sorption sites preequilibrated with water from well USGS 92). Twenty-five different mixtures were created, which ranged from 1 percent of water from well USGS 112 (and 99 percent of water from well USGS 92) to 99 percent of water from well USGS 112 (and 1 percent of water from well USGS 92). The two types of simulations were run with or without specification of calcite (and chalcedony) equilibrium and with the ANSTO or the EQ3/6 thermodynamic data bases.

Results of the various isotherm simulations (figs. 5-25 and 5-26) confirm the suggestions made in the discussion of the transport simulations that the "effective" K_d for Np sorption according to the SCM is not constant and, instead, decreases with increasing aqueous Np concentrations. The results also show the significant dependence of the sorption isotherms on (1) the presence or absence of calcite equilibrium, (2) the source of the aqueous Np thermodynamic data (the ANSTO or EQ3/6 data bases), and (3) the presence or absence of water from well USGS 92 in the equilibrated systems. However, this last factor was of little importance in the simulations for which calcite equilibrium was specified. As previously observed in the transport simulations, specification of calcite equilibrium resulted in smaller concentrations of sorbed Np; use of the EQ3/6 data base instead of the ANSTO data base resulted in larger calculated concentrations of sorbed Np. Finally, the results suggest that matching the simulated isotherms with a Freundlich isotherm equation would be possible, albeit only for a given set of geochemical conditions. Any change in conditions caused, for example, by the mixing in of a background water due to normal dispersion, or to the appearance or disappearance of reactive minerals that might affect pH or Eh conditions or the concentrations of ions competing for sorption sites, would likely affect the isotherm curve, and possibly invalidate any previously obtained match of Freundlich parameters.

5.6 Evaluation of the uncertainties associated with selected K_ds

The K_ds for Am, U, and Pu selected for the IRA model were determined using only one ground-water composition and one composite interbed sediment sample. It has been shown in chapter 4 and in earlier sections of chapter 5 of this report that K_ds for actinides can be highly dependent on the chemical and physical properties of the aqueous and solid phases. Also important is how well the laboratory experimental conditions simulate processes operating in the field. There are not enough data from WAG-7 to quantify all the uncertainties associated with the K_ds for Am, U, Np, and Pu used in the IRA model; however, some generalities can be formulated to estimate how much these K_ds could vary with changing chemical and physical properties.

The effect of aqueous chemistry on actinide sorption depends on both the actinide and its oxidation state. For example, Np(V) is the dominant oxidation state under the oxidizing conditions at WAG-7, and the primary species adsorbed is the cation NpO_2^+. Adsorption increases with pH as the surface becomes more negatively charged. The increase is most dramatic at lower pH values and begins to plateau near 8. Because the measured pH of perched water and ground water near WAG-7 ranges between 7.8 and 8.4, these changes would be expected to have only a minor effect on Np adsorption. $CaCO_3$ complexes of Np also would have some effect on sorption. As CO_3^{-2} concentration increases, the concentration of $NpO_2CO_3^-$ and $NpO_2(CO_3)_2^{-2}$ increases, thereby decreasing the concentration of NpO_2^+.

The thermodynamic modeling data for 11 perched-water and ground-water samples from the INEEL (table 4-7) show that relatively small changes in chemical composition can affect sorption when all other properties of the modeled system remain constant. These data are presented as molar ratios of total sorbed to total aqueous (K_r). For Np, K_rs ranged from 164 to 215. These values are dependent on the types of sorbing surface. For example, increasing the concentration of surface sites from 5.6×10^{-6} to 1.0×10^{-2} mol per kg H_2O would increase the Np and Pu K_rs by 2,000. These calculated K_rs also can vary with the data base used in the modeling.

Pu(V) is predicted by thermodynamic modeling to be the dominant oxidation state in water at the INEEL (table 4-6). Pu forms very strong complexes with $CaCO_3$. In fact, most of the Pu(V) in the 11 perched-water and

ground-water samples from the INEEL was calculated to be $PuO_2CO_3^-$. Because of this, sorption of Pu was computed to be minimal (table 4-7). However, the concentration of surface sites used in this model is possibly smaller than would be expected in the aquifer.

The K_d for Pu selected for the IRA model was 5,100 mL/g. The concentrations of most constituents in the synthetic ground water used in this experiment were smaller than those in most of the perched water and ground water at the INEEL (table 4-4). For example, the CO_3 concentration (96.6 mg/L) was comparable to that of the modeled ground water from well USGS 89 (table 4-4). Sorption of Pu also was greatest in this water (table 4-7). Thus, for ground water with a larger CO_3 concentration such as that from well USGS 19, the thermodynamic model indicates that the amount of Pu sorbed could decrease by 55 percent. Caution is needed when thermodynamic modeling results are extrapolated to field conditions; however, such an exercise does illustrate the uncertainty in a single K_d measurement.

Sorption of U also is dependent on the aqueous chemical composition. For example, figure 4-2a shows that a two-order-of-magnitude increase in U concentration results in a one-order-of-magnitude decrease in K_d. Increasing the ligand concentration can significantly reduce sorption of U (fig. 4-2c). Figure 4-6 shows that slight changes in pH can have a dramatic effect on the amount of U sorbed. Modeling U sorption for the 11 INEEL water samples in table 4-4 resulted in K_rs ranging from 7 to 211 for a goethite sorbent (table 4-2). Generally, sorption decreased with increasing pH and CO_3 content.

The type of surface site and value of pH also have a considerable effect on Am sorption (fig. 4-4). Formation of Am CO_3 complexes increases with CO_3 concentration resulting in less sorption. For the 11 different INEEL water samples that were modeled, K_rs varied by 400 percent.

Spatial variability in the composition of the sorbent also will have an effect on K_ds. Two important measures of sorption capacity are (1) the CEC, likely to be important for cations such as Am, and (2) the concentration of Fe oxides, likely to be important for sorption of Am, U, Np, and Pu. The K_ds selected for the IRA model (Dicke, 1997) were determined for a composite interbed material with a CEC of 17.4 meq/100 g and an Fe oxide content of 1.77 percent (Newman and others, 1995). These K_ds can be expected to decrease or increase depending on the CEC and Fe oxide content of other sediments. Bartholomay and others (1989) compiled a list of CEC measurements from previously published reports of the USGS. The data include measurements from 271 samples of interbed sediments and fracture fill from the INEEL. CECs ranged from 0.9 to 42 meq/100 g, and averaged 13.6 meq/100 g. The Fe oxide content of 11 interbed samples ranged from 0.37 to 2.86 percent (Goff, 1994). Making the assumption the K_d is linearly proportional to CEC, expected minimum, maximum, and averaged K_ds for the sediments reported in Bartholomay and others (1989) can be calculated from the K_ds determined by Newman and others (1995). These values are compared in table 5-8. The average K_ds calculated for the 271 samples are comparable to the values reported by Dicke (1997); however, K_ds can be expected to be significantly smaller in coarser sediments with smaller CEC. Conversely, K_ds will be larger in finer-grained sediments with larger CEC.

Extrapolation of the laboratory-derived K_ds used in the IRA model to field conditions at WAG-7 also could introduce uncertainty in the modeling results. K_ds measured in batch experiments can decrease as the suspended solids concentration increases (section 5.3.2.4.3). ^{90}Sr K_ds for the composite WAG-7 interbed sediment decreased by 30 percent for a 19-fold increase in the solid:liquid ratio (Newman and others, 1995). The K_ds for Am, U, and Pu for the INEEL interbed experiments were determined for solid:liquid ratios ranging from 3.5 to 150 g/L (Goff, 1994). The interbed sediments in the unsaturated zone have a solid:liquid ratio of about 4,000 g/L. Thus, it is possible that the K_ds measured in the batch experiments may not adequately represent sorption in the interbeds. Newman and others (1995) measured K_ds for U in both batch and column experiments. For crushed basalt, the column K_d was more than one order of magnitude lower than the batch K_d. For the interbed sediment, the column K_d was twice as great as the batch K_d. However, it is not possible to assess the effect of solid:liquid ratio on U sorption because of variability in pH; and, possibly because of differences in U concentration between the batch and column experiments.

A great uncertainty in the K_ds selected for the IRA model concerns possible reducing microenvironments that might be found in the source area or in more impermeable zones of the saturated interbeds. These reducing environments could strongly limit the migration of Np(IV) and Pu(IV), which are only sparingly soluble.

5.7 Summary

The primary question addressed in this chapter is, "Are K_ds for Am, Np, Pu, and U that were used in the IRA model reliable and have they been applied appropriately?" The intent in selecting these K_ds was to use technically

Table 5-8. Effect of cation exchange capacity on K_ds

[K_d, distribution coefficient; CEC, cation exchange capacity; meq/100 g, milliequivalents per 100 grams]

	K_d suggested by Dicke (1997) based on CEC of 17.4 meq/100 g	K_d calculated for the smallest CEC of 0.9 meq/100 g	K_d calculated for the average CEC of 13.6 meq/100 g	K_d calculated for the largest CEC of 42 meq/100 g
Americium	450	23	345	1,080
Neptunium	8	0.4	6.2	19
Plutonium	5,100	260	3,900	12,200
Uranium	6	0.3	4.6	14

defensible estimates for the K_ds and conservative estimates of other model parameters whenever "realistic" estimates were not available. It was not the intent of the IRA to present a worst case scenario. K_ds for Am, U, and Pu were determined experimentally; K_ds for Np were selected from the literature.

The K_d is a measure of the amount of a solute sorbed from solution by a solid phase. Advantages of the K_d approach are its mathematical simplicity and ease of obtaining experimental values. However, there are many limitations to the K_d approach. Generally, the K_d measured is a unique function of the aqueous and solid-phase compositions. This is especially true for inorganic solutes.

Thus, the K_d measured for sorption by a clay mineral will be different from the K_d measured for sorption by goethite. Competition for sorption sites is common. Increasing the concentration of competing solutes will decrease sorption of the solute of interest. Decreasing the concentration of competing solutes will have the opposite effect. Many ions form aqueous complexes with various ligands in solution. Changing the concentration of these ligands changes the concentration of the complex and alters the amount sorbed. Sorption is often pH dependent. Cation sorption increases with pH as the surface becomes more negatively charged. Anion sorption increases with decreasing pH as the surface becomes more positively charged. Changes in ionic strength of a solution can affect the electrical double layer surrounding particles to the extent that sorption properties change. If sorption is nonlinear, K_d also will be a function of the aqueous concentration of the solute of interest.

The K_d approach may adequately describe contaminant migration and reversible sorption in ground-water systems in which the aquifer regions occupied by the contaminant plume and by the background water each have uniform mineralogical and chemical compositions that remain uniform during the timescale of interest. In general, the reactive sorption of the contaminant of interest also must be adequately described by the local equilibrium assumption. The K_d approach generally will not properly describe contaminant migration in ground-water systems undergoing dynamic chemical evolution.

For the IRA model, a single composite of five sediment interbed samples was used in batch experiments to measure sorption of Am, U, and Pu from a synthetic ground water similar in composition to that from the SRP aquifer. Specific concerns regarding the K_ds recommended for use in the IRA model include the following:

(1) A literature survey of the CEC of 271 samples from the INEEL indicates that the sorption properties of aquifer solids can vary widely. Thus, although the K_ds measured for the IRA model may accurately represent sorption for the composite interbed sample used in the batch experiments, there is no guarantee that this sediment represents a technically defensible approach to estimating K_ds especially because the coarse-size fraction was eliminated from the composite samples.

(2) The assumption was made that sorption properties in the vesicles and fractures in the basalt were comparable to those in the sedimentary interbeds. Because these vesicles and fractures contain many minerals in common with the interbeds, this assumption may be valid but needs verification.

(3) The synthetic ground water used in these experiments was undersaturated with respect to CO_3 minerals, whereas most perched and infiltrating water at the SDA is

saturated or supersaturated. Because CO_3 complexes are important in the aqueous speciation of actinides, the smaller CO_3 concentration in the synthetic ground water may have resulted in overestimating sorption. There is some evidence of calcite dissolution from the interbed sediment. The pH of effluent from column experiments increased from 8.0 to 8.4, and conductivity also increased. If calcite did dissolve in the batch experiments, then CO_3 concentrations could have increased to levels comparable to those of other water at the SDA. However, there were no data from the batch experiments to evaluate this possibility.

(4) The limited data presented in the report by Newman (1995) indicate that sorption was nonlinear; therefore, the measured K_ds apply only to the range of concentrations used in the experiments. Concentrations outside this range are likely to result in K_ds that are either smaller or larger than those reported here.

(5) The K_d of 5,100 mL/g for Pu(total) recommended for risk assessment modeling is based on experimental results for Pu(V). A K_d of 110 mL/g was measured for P(VI). Therefore, the recommended K_d for Pu(total) does not meet the stated intent to maintain technical defensibility and conservatism, unless it can be shown that Pu(VI) will not be present at WAG-7. These experiments were conducted using only one initial Pu concentration. If sorption is nonlinear, then the K_d will change with Pu concentration.

(6) A K_d for U as small as 3 mL/g was measured; therefore, the recommended K_d of 6 mL/g does not meet the stated intent to maintain technical defensibility.

(7) The cause of the enhanced-mobility fraction responsible for the early elution of Am and Pu in the column experiments needs to be resolved. If this fraction represents transport as an aqueous complex, then the K_ds used in the IRA model are too large. If the radionuclides are transported as colloids, basing risk assessment on sorption-controlled transport may need to be reevaluated.

(8) Sorption also is dependent on the initial aqueous speciation of the actinide that enters the unsaturated zone from the disposal area. These species may be quite different from those used in the batch experiments. Therefore, K_ds could be much different.

(9) The experimental data from the literature used to select a K_d for Np show that sorption is highly dependent on aqueous-phase chemistry and solid-phase mineralogy. Given this dependency, it might be more appropriate to determine the sorption behavior of Np for the range of geochemical conditions specific to the INEEL. The literature K_ds that were evaluated ranged from 1 to 80 mL/g. Therefore, the K_d of 8 mL/g selected for risk assessment does not meet the intent to maintain technical defensibility and conservatism.

There are not enough data from WAG-7 to quantify all the uncertainty associated with the K_ds for Am, U, Np, and Pu used in the IRA model. The data presented in chapter 4 show that sorption of Am, U, Np, and Pu generally varies as a function of pH, CO_3 concentration, and sorption-site type and concentration. For 11 different water samples from the INEEL, thermodynamic modeling indicates that sorption of Am can vary by 400 percent, U by 3,000 percent, Np by 25 percent, and Pu by 55 percent. For a constant water composition, the K_ds selected for the IRA model could vary by as much as 1,500 percent for the range in concentration of surface sites measured in interbed sediment and fracture fill samples collected from the INEEL. In conclusion, the experimental conditions used to measure K_ds for the IRA model do not adequately represent the aqueous- and solid-phase variability at WAG-7.

6.0 Task 4: Transport model analysis

6.1 Introduction

The Interim Risk Assessment (IRA) model of water and contaminant transport, described by Becker and others (1998) and Magnuson and Sondrup (1998), supports the assessment of future risks to human health and safety from Subsurface Disposal Area (SDA) contaminants of potential concern (COPC's). The numerical basis of the model is the code TETRAD (Vinsome and Shook, 1993). Model output includes the aquifer contaminant concentrations that are the basis for estimates of effects on human health. This model is an essential element in predicting the effect of remedial options.

This review assesses the value and adequacy of this model as a tool for risk assessment. In this report, the term "IRA model" refers to the model used in the IRA to predict contaminant concentrations and the effects of hydrologic and chemical processes on the concentrations. This review does not evaluate the interpretation of these concentrations as risks to human health. A significant part of our evaluation is a comparison of model representations with the processes and phenomena explained in other parts of this report. Section 6.2 describes and reviews the IRA assumptions and simplifications used in setting up the numerical code. Section 6.3 describes and reviews specific aspects of the numerical code TETRAD and the calibration developed for it. Section 6.4 reviews the application of the model, especially with respect to its predictions and defensibility related to risk assessment.

This review also does not address issues that involve definition of the source term and modeling of contaminant release rates. It is clear that definition of the source term and release rates are at least as important as other issues related to the formulation of the computational scheme to predict actinide transport. As pointed out in the IRA, the source-term release-rate model has not been calibrated and remains a major deficiency that needs to be resolved (Becker and others, 1998, p. 5-38 and 7-12).

6.2 Review of significant Interim Risk Assessment assumptions and simplifications

The assumptions and simplifications used in modeling were described by Becker and others (1998) in the IRA, especially in the hydrologic descriptions in chapter 2 and the discussion of modeling assumptions in chapter 5. These assumptions and simplifications address the heterogeneity of the subsurface, possible transport mechanisms, and limited interaction of water and contaminants with influences outside the Waste Area Group 7 (WAG-7) domain.

6.2.1 Hydrogeologic framework—geometrical aspects

This section discusses basic geometrical assumptions related to major components of the hydrogeologic system.

6.2.1.1 Definition and description of the model domain

In plan (horizontal) view, the SDA occupies an area with dimensions of about 1,500 m in the x direction (east to west) and as little as about 250 m to as much as about 750 m in the y direction (south to north). The additional consideration for modeling the transport of organic constituents effectively increased the modeled area to robust dimensions of 9,000 by 9,000 m (fig. 6-1).

In vertical cross section, the numerical simulator includes both the unsaturated and saturated zones. The unsaturated zone is assumed to be 175 m thick, and the saturated zone about 76 m thick. The assumed thickness of the Snake River Plain (SRP) aquifer, 76 m, is consistent with the WAG-3 and WAG-10 modeling studies (Becker and others, 1998, p. 5-66) and is supported in studies by Rodriguez and others (1997), McCarthy and others (1995), and Robertson (1974). As noted in chapter 2, these are among the smallest estimates of thickness for the SRP aquifer. Therefore, this assumption is probably conservative for predicting dilution of contaminants in the aquifer; however, dispersion and advective mixing processes in the saturated zone are not well characterized.

The plan view and vertical cross-section dimensions define a study volume that is 81 km^2 and 251 m thick, or about 20 km^3. This block is the model domain. Within the model domain, an area of local grid refinement is defined that is 3,000 m in the x direction and 2,000 m in the y direction. Almost all of the data available for modeling are from the region of this smaller sub-domain (fig. 6-1).

The land surface is treated as if it were perfectly flat (Magnuson and Sondrup, 1998, p. 2-6). Although actual deviations from flatness are likely the main local influence on infiltration rates at the SDA, the effects of these topographic deviations are incorporated into the infiltration rates estimated by Martian (1995, p. 31) and used in the IRA model. Because there are likely no other major effects of the flat-surface assumption, its use in the model likely does not significantly affect model predictions.

The surficial sediments and sedimentary interbeds (A-B, B-C, and C-D) are assumed to have spatially variable geometric surfaces and thicknesses that affect water and contaminant movement (Becker and others, 1998, p.

5-65). Although this assumption is clearly true, the specific means of representing these lithologic units in the IRA model could underestimate the degree and hydrologic effect of this variability. Uncertainties associated with this assumption are discussed further in section 6.2.1.2 on geostatistical applications. In particular, the kriging techniques used to treat this variability inherently entail smoothing that may misrepresent geometric features that deflect or concentrate water and contaminant transport. However, information that would permit a detailed treatment of these geometric features is not available and possibly not obtainable by any practical means.

Interbeds below the C-D interbed are assumed to be thin and discontinuous and to have no significant effect on flow and contaminant transport near the SDA (Becker and others, 1998, p. 5-65). In actuality, these lower interbeds are discontinuous, but they could be substantial in places (Anderson and Lewis, 1989, p. 24–31). Discontinuous interbeds could generate additional preferential flow (Magnuson and Sondrup, 1998, p. 6-5 to 6-6), for example, by the mechanism of funneled flow, but in the absence of this mechanism, they affect flow similarly to the more continuous interbeds. Although preferential flow is not treated explicitly in the model, because there are probably greater causes of preferential flow in the unsaturated zone and because interbeds are the primary sorbing media for the actinides and have a generally impeding effect, the exclusion of these units from the model probably is conservative.

6.2.1.2 Geostatistical applications

The subsurface lithology at the SDA consists of a discontinuous layer of surficial sediments that is underlain by a series of basalt flows separated by discontinuous but mappable interbeds of alluvial and eolian sediments (A-B, B-C, and C-D interbeds). The surficial sediments and interbeds correspond to the horizons of enhanced resolution in the vertical discretization of the model domain as presented by Magnuson and Sondrup (1998). The positions of the interbeds are known from borehole information that defines the elevation of the top of a given interbed and, in cases of complete penetration, its thickness. Geostatistical techniques were used to interpolate the top elevation and thickness of the three primary interbeds and the surficial sediments through the grids that discretize the model domain. A review and some extension of the geostatistical techniques used in the IRA model are presented below. This work starts from the basic geostatistical analysis of Magnuson and Sondrup (1998) and reviews the results of decisions made in their analyses and interpretations. Although this review is mostly qualitative, quantitative evaluation of results are presented. The qualitative review includes a discussion of the procedural steps used in the IRA and implications inherent in geostatistical applications. The quantitative evaluations are based on cross-validation statistics that are presented in maps and tables that describe kriging standard deviations. Much of the information presented in these evaluations originated in this review because cross validation and kriging standard deviations were not reported by Magnuson and Sondrup (1998).

The data used for these quantitative evaluations were residuals obtained from detrended raw data presented in table 2-1 of Magnuson and Sondrup (1998, p. 2-2 to 2-4). The detrending procedure is briefly described and discussed below. It is important to note that the kriged estimates were not added back to the spatial trend, or retrended in our quantitative evaluations to describe variability and confidence in the kriged estimates. The number of data points available for fitting variogram models of the thickness and top elevation of the surficial sediments and sedimentary interbeds was different for each of these units. However, the number of points available for each lithologic unit was sufficient for adequate definition of most sample variograms. However, the distribution of data limit the spatial representativeness of defined sample variogram points. All data, except those for a few widely spaced points within the larger expanse of the 9,000 by 9,000 m model domain, were collected within the SDA. This necessitated the assumption that the values of the variograms defined at lags within the SDA also apply in the general model domain if the variograms are to be used in these areas. Conversely, definition of the variograms at larger lags was problematic because of the lack of data locations at these lag values.

The geostatistical analyses for each of the eight variables (top elevation and thickness of the surficial sediments, and the A-B, B-C, and C-D interbeds) consisted of three steps:

(1) defining a polynomial drift or spatial trend for each variable (top elevation and thickness) and removing this trend to develop residuals that formed the data set for the remainder of the kriging analyses (detrending the data),

(2) construction of variograms for the data set of residuals for each variable, and

(3) kriging the residuals, using ordinary kriging, to grid locations and adding back the trend values computed for these locations (retrending the data).

Although justification for defining spatial trends was not readily apparent, the equations describing the trends were kept to low-order polynomials by Magnuson and

Sondrup (1998), as is generally recommended. In addition, as part of this review, the relation between the resultant residuals and the x and y coordinates were found to be free of trends. The use of residuals introduced the possibility of universal kriging as an alternative to ordinary kriging, which would have negated the need for retrending. It is not expected that the use of universal kriging methods would produce any changes to the results. Use of these alternative methods is simply mentioned because retrending and detrending procedures are handled in the actual kriging process rather than with pre- and post-processing steps.

The kriged top elevations for the surficial sediments and the three interbeds were used to place each lithologic unit in the vertical grid. The kriged thicknesses were used to describe spatial variation in the horizontal grid and to distribute the vertical thickness. It is important to note, as Magnuson and Sondrup did (1998, p. 2-9), that known areas of zero thickness were superimposed onto the kriged thickness results. The need for this is discussed in section 6.2.1.2.2.

6.2.1.2.1 Variogram construction

The variogram model and parameters for each variable are given in table 6-1 and figures 6-2 through 6-5. All variograms have stationary models within their ranges and are described by spherical, exponential, or Gaussian forms. Nugget values range from 0 to 1.6 m^2. Most of the sill values apparently were set to the variance of the residual data sets. This systematic procedure is not uncommon. It slightly simplifies variogram modeling in that the sill is not estimated from the sample variogram points but instead is set. The effects of this procedure on results in this study are practically insignificant.

Figure 6-2b shows the variogram used by Magnuson and Sondrup for the thickness of the surficial sediments. The range of 172 m for the surficial sediment thickness reported by Magnuson and Sondrup (1998), the smallest range of any of the eight variables, is also the range they used to model the variogram. The reported ranges of all other variables (Magnuson and Sondrup 1998), except for that of the C-D interbed thickness (also used to model the variogram), are one-third of the ranges used in this review and appear to be correlation lengths. The correlation length often is cited in the literature as being a conservative range and is approximately one-third of the range used to fit the sample variogram points. Some subjective adjustment of the variogram model, such as increasing the sill or range or both, is possible. For this reason, values for the sill and range (adjusted for correlation length) reported in table 6-1, differ slightly from table 2-2 by Magnuson and Sondrup (1998). However, it is important to note that even the most optimistic adjustment would only nominally increase the range. In a strict sense, that assumes spatial variability is well characterized within the range, additional information collected from the field can provide increased variogram range if it is collected from points located farther than the variogram range of existing point information.

The extent of the ranges of most variables in the variogram are such that kriging analyses for areas near the SDA can be an effective estimation procedure, implying that the advantages of kriging over other estimation techniques will be realized. Figures 6-2a and 6-5a show the variograms for the top elevations of the surficial sediments and the C-D interbed. Ranges for top elevations for these variograms, in contrast to those for the thickness of the surficial sediments and the C-D interbed are extended, which allows estimation of the top elevation over a much larger area. These variograms also are unusual with respect to their cross-validation statistics, as discussed below.

Outside the SDA but within the model domain, the spatial distribution of data (residuals) points for most variograms relative to the ranges of variables in the variogram eliminates kriging's special advantages in distributing spatial information; therefore, kriging becomes ineffective and estimation defaults to simple averaging of available data. Some indication of this is evident in the summary statistics presented in table 6-1, as discussed below.

The variograms for each variable were evaluated by a kriging cross-validation technique in which a data point for a location is omitted from the data set and kriging results for that location are obtained by using the subset of remaining values. The procedure is repeated for each value in the data set. Therefore, each data location will have a kriging estimate, a kriging standard deviation, and a data value. Statistics obtained from cross validation include (1) a mean estimation error defined as the difference between the data value and the kriging estimate, and (2) a root-mean-squared error ratio defined as the estimation error divided by the kriging standard deviation. Acceptable variograms are those for which cross-validation indicates a mean estimation error near zero (ensuring unbiasedness), a minimized root-mean-squared error (ensuring a small error estimate), and an average reduced root-mean-squared error near unity (ensuring consistency in the estimation accuracy).

Table 6-1. Variogram models, parameters, and cross-validation statistics for thickness and top elevation variables for surficial sediments and interbeds A-B, B-C, and C-D

[Units for nugget and sill are meters squared; units for range, mean error, and root-mean-squared error are meters; ranges reported in this table were adjusted by a factor of 3 to compensate for presumed reporting of correlation length by Magnuson and Sondrup (1998) except ranges for the thickness of surficial sediments and the C-D interbed, which were reported as true ranges. Sample numbers shown in parentheses () for the thickness variable indicate the number of samples within the total sample set that represent partial penetration of the interbed. These values are reported as greater than the penetrated thickness by Magnuson and Sondrup (1998, table 2-1)]

			Parameters			Cross-validation statistics		
Variable	Number of samples	Variogram model	Nugget	Sill	Range	Mean error	Root-mean-squared error	Reduced root-mean-squared error
Surficial sediments								
Thickness	94	Spherical	1.30	3.90	176	0.037	1.621	0.868
Top elevation	94	Gaussian	0.80	20.30	3,900	0.170	3.443	1.424
A-B interbed								
Thickness	94 (1)	Exponential	0.15	1.03	330	0.035	0.603	0.841
Top elevation	44	Exponential	0.00	5.50	350	0.317	1.268	1.136
B-C interbed								
Thickness	91 (3)	Exponential	1.60	5.10	480	-0.090	1.918	1.018
Top elevation	91	Exponential	0.20	2.80	450	0.050	1.045	1.052
C-D interbed								
Thickness	76 (22)	Spherical	0.00	8.50	205	-0.078	2.839	2.244
Top elevation	76	Gaussian	1.00	11.00	2,900	0.395	3.120	1.536

The cross-validation statistics are shown in table 6-1. The results indicate that the mean estimation errors for some variables are smaller than the absolute value of 0.10 m. For this study, these smaller values are relatively good. Mean errors for three of the four top elevations are larger than 0.10 and, for the C-D interbed, are about 0.40. The reduced root-mean-squared errors usually are considered acceptable if they are within an interval defined as follows:

$$1 \pm 2\sqrt{\frac{2}{\text{number of samples}}} \qquad (6.1)$$

Using this reduced root-mean-squared error criterion for the variograms for the top elevation of the surficial sediments and the top elevation and thickness of the C-D interbed variables should be considered less than optimal for the region encompassed by the model domain (9,000 by 9,000 m).

6.2.1.2.2 Kriging results

The kriging standard deviation, a product of kriging theory, is a function of the geometry of the data points implemented through the variogram that is used for obtaining a kriging estimate. It is also a measure of the uncertainty associated with a kriged estimate; therefore, the kriging standard deviation is also a measure of confidence. Maps of kriging standard deviations often are presented with maps of kriging estimates so that the areas where kriging is most effective and where it is ineffective can be seen. Kriging standard deviation maps were prepared as part of this review for all variables and the results are summarized in table 6-2 and illustrated in figures 6-6 through 6-21.

Table 6-2 shows that for all variables except two (the top elevations for the surficial sediments and the C-D interbed), the kriging process was ineffective throughout about 90 percent of the 9,000 by 9,000 m model domain. In other words, although the kriging process was capable of making estimates, most of the estimates were based on simple averaging of data. In contrast, at the SDA, which represents about 5 percent of the model domain, all variables, except perhaps the top elevation of the A-B interbed (fig. 6-10) and the thickness of the C-D interbed (fig. 6-20), were effectively characterized.

Figures 6-7 and 6-9 represent the extremes for all the characterizations. The results for the top elevations of the surficial sediments, which came from a variogram with one of the longest ranges (fig. 6-1), portray relatively high confidence in kriged estimates for most of the 9,000 by 9,000 m model domain. The results for the thickness of the surficial sediments, which came from the variogram with the shortest range (fig. 6-1), portray the highest confidence in kriged estimates for most of the SDA area; however, the full advantages of kriging were not realized for most of the model domain. These areas are characterized as those of ineffective kriging in this review and correspond to areas that are farther from any measured values than the particular variogram range.

In summary, the range of the variograms is an important factor in determining how much of the model domain will be characterized effectively by kriging. For the variables kriged by Magnuson and Sondrup (1998), only two, the top elevations for the surficial sediments and the C-D interbed, were characterized effectively for more than about 10 percent of the 9,000 by 9,000 m model domain. However, the kriging for the other variables was generally effective for most of the SDA. For areas where kriging was ineffective, estimates are essentially equivalent to those obtained from simple averaging.

It is also important to note that the kriging process introduces smoothing into the resultant estimates; therefore, for estimates of thickness, kriging will extend areas of nonzero thickness into areas of zero thickness. To preserve known gaps in the sedimentary interbeds in the SDA, Magnuson and Sondrup (1998, p. 2-9) superimposed areas of zero thickness onto kriging results.

6.2.2 Nature of materials

The effect of particular subsurface materials on water and contaminant transport is represented quantitatively in the IRA model by specific hydrologic characterizations. Table 6-3 summarizes the basic model components involved, with information on the types of measured or estimated data used to characterize them.

Magnuson and Sondrup (1998, p. 2-9) noted that the hydraulic properties used in the IRA model were delineated on the basis of lithology, and thus that their simulation represents "only contrasts in hydraulic properties between dissimilar media (sediments and fractured basalts)". This implies the assumptions that (1) the hydraulic properties correlate strongly with directly observable features of the subsurface media, and (2) the properties are homogeneous within each lithologically identifiable layer. These assumptions allow the grouping of property characterizations (by various means) within a geomorphologically distinguishable layer. Given the small number of available measurements, these kinds of assumptions are unavoidable in the current (1999) modeling efforts, but they create serious problems in determining the reliability of model results.

Table 6-2. Relative confidence in kriging estimates

[Confidence range, relative confidence in kriging estimate expressed as a percentage of maximum confidence; ineffective kriging applies to areas where the kriging process is equivalent to simple averaging]

Variable	Confidence range				
	0 to <25	25 to <50	50 to <75	75 to 100	Area of ineffective kriging
	Fraction of model domain in specified lithologic unit				
	Surficial sediments				
Thickness	0.02	0.01	0.01	0.00	0.97
Top elevation	0.08	0.22	0.36	0.33	0.00
	A-B interbed				
Thickness	0.05	0.02	0.01	0.00	0.92
Top elevation	0.03	0.01	0.00	0.00	0.95
	B-C interbed				
Thickness	0.08	0.03	0.02	0.01	0.86
Top elevation	0.07	0.03	0.01	0.00	0.89
	C-D interbed				
Thickness	0.02	0.01	0.01	0.00	0.96
Top elevation	0.10	0.21	0.36	0.33	0.00

Table 6-3. Summary of hydrologic characterizations used in the Interim Risk Assessment (IRA) model (Magnuson and Sondrup (1998, see especially table 2-4). Some characterizations were adjusted in the IRA model calibration, see table 6-6, section 6.3.2 of this report)

[IRA, Interim Risk Assessment; SDA, Subsurface Disposal Area; K_{sat}, saturated hydraulic conductivity; WAG, Waste Area Group; LSIT, Large Scale Infiltration Test; COPC's, contaminants of potential concern]

Hydrologic characterization for the IRA model	Basis of evaluation	Estimated quantities	Comments
Flow properties of surficial sediments	Neutron-measured transient water contents in 17 holes in the SDA (Bishop, 1996; Martian, 1995, UNSAT-H calibration)	K_{sat}; van Genuchten-Mualem unsaturated flow parameters	The model as constructed has little direct sensitivity to these because infiltration/recharge/runoff effects are treated separately in the infiltration model
Infiltration in the SDA (combined effects of climatic and hydrogeologic properties)	Neutron-measured transient water contents in 17 holes in the SDA (Bishop, 1996; Martian, 1995, UNSAT-H calibration)	Spatially and temporally variable infiltration rates at the SDA	Only two holes are in disturbed soils; uncertain contributions from historic floods; calibration data from 1994 and 1995 only
Flow properties of interbed sediments	WAG-3 modeling estimates; core-sample characterizations by Magnuson and McElroy (1993)	K_{sat}; van Genuchten-Mualem unsaturated flow parameters	Available data do not permit characterization at the level of accuracy and detail relevant to contaminant transport
Flow and transport properties of basalts in the unsaturated zone	Water and tracer data from the LSIT	Horizontal and vertical permeability; fracture porosity; longitudinal dispersivity	Selective use of data from the LSIT that supported use of a radially symmetric porous-media equivalent model
Flow properties of basalts in the saturated zone	WAG-10 model results; pump-test data; potentiometric-surface data	Horizontal permeability	Selective use of hydraulic head data; limited hydraulic head data to define boundary conditions; neglect of possible effects of spreading areas; determination only of ratios of permeabilities from different units
Contaminant transport properties of COPC's	Measured concentrations of contaminants in the aquifer	Distribution coefficients; specific-surface areas and apertures of fractures in basalts	Source-term uncertainty; use of nondetects in calibration

6.2.2.1 Means used to determine hydraulic properties

The means available to determine hydraulic properties usually involve a tradeoff between quality of results (especially directness and accuracy) and cost or convenience. Studies of large and complex regions of the subsurface, like that of the SDA, usually rely heavily on indirect methods (for example, inverse modeling, as discussed below) that typically provide results on a larger scale but with less resolution and less reliability than more direct methods. In some cases, data from more direct means are available. For example, water retention of surficial sediment cores (Shakofsky, 1993, 1995), can be measured directly, either in situ or with extracted samples. These kinds of direct measurements usually do not represent the entire range of relevant media or conditions, so it is frequently necessary to interpolate or, less desirably, to extrapolate. These procedures could be used, for example, to estimate the needed properties at different water contents or spatial positions. Another practical use of direct measurements is comparison with inverse-model results to determine whether the measurements support or invalidate the more voluminous but lower quality modeled results.The adaptation or adjustment of measurements from one medium to another, although generally less reliable than direct measurements, is adequate for some purposes. For example, hydraulic conductivity measurements for a coarse sand can be adjusted by scaling methods (Miller and Miller, 1956) to estimate the hydraulic conductivity of a similar, but finer, sand. There also are methods available for predicting certain properties from other, easier-to-measure properties. In unsaturated zone hydrology, one of the most widely used types of such methods is based on capillary bundle models (Childs and Collis-George, 1950; Mualem, 1976) that predict unsaturated hydraulic conductivity from water retention. A method of this type can be used in combination with the assumption by Magnuson and Sondrup (1998) that hydraulic properties can be based on lithology rather than individual measurements.

Most of the methods used for estimating the hydraulic properties of the various subsurface materials at the INEEL involve some form of inverse modeling. For example, the field-scale hydraulic properties of the fractured basalts were assumed to be adequately described by the inverse model results by Magnuson (1995) for the Large Scale Infiltration Test (LSIT) (Becker and others, 1998, p. 5-66). The basic scheme of inverse modeling is the systematically repeated use of a forward model, which predicts a measurable quantity (for example, water levels in a well as a function of time) from fundamental properties of the system (for example, hydraulic conductivity) and particular input conditions (for example, infiltration as a function of time). Inverse modeling is used when the predicted quantity is already known, but the fundamental properties of the system are not. The forward model calculations are repeated with systematically varied trial values of the fundamental properties, so that the property values that lead to the most accurate output can be identified and taken as system characteristics. One common pitfall is that the results are not necessarily unique—more than one combination of input property values can lead to essentially the same output, so the system characteristics identified may not be the best possible. For example, if a deficiency in one property or in some aspect of the model framework compensates for another deficiency that has an opposing effect, then the result of the inverse modeling will be fundamentally defective in a way that may not be apparent. The reliability of inverse modeling results depends strongly on the appropriateness of applied assumptions and simplifications, for example, those concerning surface-water ground-water connections, multimodal porosity, anisotropy, and matrix diffusion. Reliability of results also requires that all significant phenomena related to contaminant transport are represented in the data used for the calibration. For example, time and space intervals and the type of measurements must not be insensitive to hydrologic processes of significance. Model calibration (discussed for the IRA model in section 6.3.2) generally involves inverse modeling in which a particular data set is chosen as a target or standard for the predicted quantities.

6.2.2.2 Fractured basalts in the unsaturated zone

Some assumptions included in the IRA model are that in the fractured porous basalts, flow is controlled by the fracture network and that the basalts can be represented adequately as equivalent to a high-permeability, low-porosity medium (Becker and others, 1998, p. 5-66). As discussed in chapter 2, such consideration of fractured media as equivalent to granular media is common. This assumption means, however, that all important transport phenomena must be encompassed by the equivalent medium. For purposes of predicting travel times, this assumption is a basic deficiency in the model and, therefore, is not a conservative assumption. Because spatially averaged behavior is inherent in the equivalent-granular-medium assumption there will be some flow paths with markedly faster transport than this assumption predicts. Unless the amount of contaminant transport in such preferential-flow paths is negligible because of factors such a dilution in the subsurface, this assumption will lead to

underpredictions of contaminant concentrations at certain points away from the source.

Various algebraic formulas can represent hydraulic properties of the medium that is taken as equivalent to the fractured, porous basalts. The IRA model uses the Brooks-Corey (1966) and van Genuchten (1980) empirical formulas for water retention curves. For the relative permeability/saturation and saturation/water potential relations for the fractures in the basalts it uses the Brooks-Corey formulas (Brooks and Corey, 1966). Both of these relations were developed and tested for use with soils, not fractured rock. However, there is precedent and support for their use with fractures, for example, the use of the Brooks-Corey formula to represent water retention in single fractures (Reitsma and Kueper, 1994). A van Genuchten curve resembles a Brooks-Corey curve but differs mainly in having a rounded rather than a sharp bend at the part of the curve representing the transition from saturation to unsaturation. Thus a van Genuchten curve could represent water retention in a fracture. For an assemblage of fractures, as in a macroscopic chunk of basalt, the resulting hydraulic properties probably would be represented reasonably by these formulas, but because the curve near the saturated-unsaturated transition probably would be more smoothly rounded, the van Genuchten formula could be a better representation. These formulas might be as suitable for fractured basalts as for soils, but for either type of medium, these representations sometimes deviate substantially from the actual properties. This deviation, which typically is a problem, for example, when the dry range is important (Nimmo, 1991), is currently a topic of controversy in the hydrologic community. Liu and others (1998) concluded that because not all fractures actively conduct water, the processes involved in conducting flow by only a few fractures "may require formulating the fracture water flow in a different way." They also noted that "Specifically, the van Genuchten (1980) and other relations... may not be valid for describing fracture water flow without suitable modification or generalization." Magnuson and Sondrup (1998, p. 2-25) also acknowledged this by noting that "Determining constitutive relationships for fractures continues to be an active research area."

The hydrogeologic properties of basalts in the unsaturated zone, (the permeability (k), anisotropy (k_v/k_h), the fracture porosity (n_f), the longitudinal dispersivity (V_L), and the Brooks-Corey parameters for unsaturated water retention and relative permeability), were determined by inverse modeling to data collected during the LSIT (Magnuson, 1995; Dunnivant and others, 1998). The LSIT was conducted by ponding water on the ground surface in a 183-m-diameter basin and monitoring for the arrival of water and conservative and reactive tracers in wells located on lines radiating outward from the center of the basin and in rings located 15, 90, and 230 m from the edge of the basin. Magnuson and Sondrup (1998) further refined the parameter values using limited borehole data on the distribution of perched water beneath the SDA and changes in the elevation of perched water over time (section 6.3.2).

Estimates for values of properties of the basalts used in the simulations by Magnuson and Sondrup (1998, table 2-4) were taken from a variety of sources. Values used as initial estimates of permeability for basalts in the unsaturated-zone portion of the model were taken from Magnuson (1995, table 4). Based on perched water-level changes directly beneath the circular infiltration pond and water-level changes at observation wells located at varying distances from the pond, Magnuson estimated the vertical permeability (k_v) to be 300 mD and the horizontal permeability (k_h) to be 90,000 mD. Magnuson (1995, p. 38) recommended a porosity of 0.03 and a k_v of 175 mD to best match B- and C-ring hydrographs and B-ring breakthrough curves in the LSIT. The values used in the IRA model for porosity and k_v, 0.05 and 300 mD, respectively, were not entirely consistent with the inverse-model results of the LSIT. Magnuson and Sondrup (1998) found it necessary to decrease k_h to 9,000 mD to recreate perched-water conditions beneath the SDA. Larger values of k_h allowed modeled percolation from the SDA to migrate rapidly downdip, and prevented the observed perched-water lenses from being simulated. The permeability estimates considered by Magnuson and Sondrup (1998) are presented in table 6-4.

The relation between relative permeability and saturation for basalts was assumed by Magnuson and Sondrup (1998) to be linear. Magnuson (1995) showed that the simulated water movement in the basalts beneath the basin of the LSIT was somewhat sensitive to the curvature in the assumed relative water-permeability/water-saturation relation; as the curvature in this relation increased, the rate of water movement slowed because the fractures had to fill to a large extent before their permeability increased sufficiently to transmit the infiltrating water (Magnuson, 1995, p. 32–37). Magnuson (1995) concluded, probably correctly, that the rate of water movement was more sensitive to the absolute (saturated) permeability than to the unsaturated hydraulic characteristics of the fractures.

Table 6-4. Estimated permeability of fractured basalts at the Subsurface Disposal Area (SDA) considered for use in the Interim Risk Assessment model

[WAG, waste area group; k, permeability; mD, millidarcy; k_v, vertical permeability, k_h, horizontal permeability]

WAG-10 model	SDA saturated-zone model	Large-Scale Infiltration Test	SDA unsaturated-zone model
k_{zone53} = 168,000 mD	k_{low} = 153 mD	k_v = 300 mD	k_v = 300 mD
k_{zone54} = 1,800,000 mD	k_{medium} = 16,300 mD	k_h = 90,000 mD	k_h = 9,000 mD
	k_{high} = 1,200,000 mD		
	k_{basalt} =85,000 mD		

As Magnuson and Sondrup (1998) noted, data on the unsaturated hydraulic characteristics of fractures are extremely limited; however, several theoretical studies indicate that the relation between water relative permeability and water saturation is nonlinear (for example, Kwicklis and others, 1998, figs. 17 and 18c). Based on the sensitivity analysis performed by Magnuson (1995), the effect of including a nonlinear relative permeability relation in the simulations would be a calibrated absolute permeability larger than otherwise would be calculated in order to compensate for the relatively small fracture permeability associated with the nonlinear curves at partial saturation. Alternatively, the effect of including a nonlinear relative permeability/saturation relation would be to hold the perched water beneath the SDA with a larger absolute permeability for the basalt (Magnuson and Sondrup, 1998).

Both Magnuson (1995) and Magnuson and Sondrup (1998, p. 2-26 to 2-27) assumed a value of 32 kPa for the Brooks-Corey fitted parameter for matric-potential scaling (A_{aw}). This implies that the average fracture aperture is 47 x 10^{-6} m (47 μm), based on the capillary rise equation adapted for parallel-plate fractures (Kwicklis and Healy, 1993):

$$P_c = \Delta\rho g h = 2\sigma\cos\Theta b_f \qquad (6.2)$$

where:

P_c = capillary pressure (32,000 Pa);
ρ = density of water (997.0 kg/m^3 at standard temperature);
g = gravitational acceleration (9.81 m/s^2);
h = height of capillary rise (m);
σ = interfacial surface tension between water and air (75 x 10^{-3} N/m at standard temperature);
Θ = contact angle between the media and the water (typically assumed to be 0 for silica-based glasses); and
b_f = fracture aperture (m).

In determining the fracture surface area for the basalts, Magnuson and Sondrup (1998, p. 5-6) assumed that the fracture porosity (ϕ_f) of the basalts is 0.05 and that the fracture apertures are 0.001 m (1,000 μm), considerably larger than the 47 μm apertures implied by the assumed A_{aw} value of 32 kPa, as noted above. The Magnuson and Sondrup values of ϕ_f and b_f imply that there are ϕ_f/b_f = 50 fractures per m^3 assuming that each fracture extends over a 1-m^2 area within a 1-m^3 volume. If there are, for example, 3 mutually orthogonal fracture sets, then about 34 fractures per cubic meter contribute to permeability in any direction. Calculated from the cubic law, the permeability of a single fracture, k_f, is:

$$k_f = b_f^2/12 = (0.001)^2/12$$

$$k_f = 8.3 \times 10^{-8} m^2 \qquad (6.3)$$

and the fracture continuum permeability (k_{fc}) may be calculated as:

$$k_{fc} = (34)(8.3 \times 10^{-8} m^2)(0.001 m/m)$$

$$k_{fc} = 2.8 \times 10^{-9} m^2 \qquad (6.4)$$

This value of k_{fc} is approximately 2,800 D or 2,800,000 mD, a value that is much larger than the k_{fc} value of 9,000 mD that Magnuson and Sondrup used in the model.

In summary, the modeled hydraulic properties of the basalts are highly simplified with respect to actual characteristics. When interpreted on the basis of simple parallel-

plate models, assumptions about the capillary properties, porosity, aperture and permeability of the fractured basalts are not entirely consistent with each other. Although these inconsistencies do not necessarily negate the conclusions of the study, improved internal consistency would give more credence and rigor to the results.

6.2.2.3 Surficial sediments

The IRA model relies for hydraulic properties of the surficial sediments on averages of Martian's (1995) inverse model results fit to neutron data from 17 shallow boreholes in the SDA. The laboratory measurements of Shakofsky (1995), summarized by Shakofsky and Nimmo (1996) and updated by Nimmo and others (1999), are useful for comparison with the inverse model results because these direct measurements were made on core samples from undisturbed soil and a simulated waste trench near the SDA. The model results differ from direct measurements in that (1) the inverse-modeled K values of Martian (1995) tend to be smaller by an order of magnitude or more, and (2) water retention remains near saturation at more extreme values of matric pressure. The second difference could also be described by saying that the Martian curves have air-entry pressures farther from zero matric pressure.

Small K might mean that the model tends to underestimate flow rates. Air-entry pressures farther from zero might mean that the model tends to overestimate the amount of soil that is near saturation (and hence would have faster flow). At any given time, these deviations might compensate for each other to some degree, but the net effect is not predictable from available information.

The hydraulic properties of the surficial sediments relate to the local hydrology in many respects. The surficial sediments are not considered to substantially impede contaminant transport, so flow rates within them probably are not a major influence on the modeled concentrations relevant to risk assessment. The properties are closely related to infiltration and recharge, but treatment of these factors in the model does not depend directly on the estimated hydraulic properties of the surficial sediments.

Another assumption is that waste at the SDA has the same hydraulic properties as the surficial sediments (Becker and others, 1998 p. 5-65). Although this is obviously not true, it is a reasonable assumption in the sense that it should not affect the WAG-7 modeling significantly. Hydraulic properties of the waste could affect source releases, but the model treats this factor in terms of the release rate in the source term. Wastes are a small fraction of the volume of the surficial layers and (except for being the source of contaminants) are not likely to significantly affect contaminant transport. The disturbances caused in the process of burial can significantly affect the hydraulic properties of the surficial sediments (Andraski, 1996; Shakofsky and Nimmo, 1996), but again, such effects are treated indirectly in the infiltration model.

6.2.2.4 Sedimentary interbeds

In a general way, properties and possible transport modes of the interbeds are similar to those of the surficial sediments. In part because they are less accessible, the interbeds have been even less completely characterized in terms of hydraulic characteristics and heterogeneity than the surficial sediments. The hydraulic properties of the sedimentary interbeds are assumed implicitly in the IRA to be adequately represented as equivalent to those of a homogeneous, isotropic, granular porous medium in which the flow is not preferential.

Magnuson and Sondrup (1998, p. 6-5) summarized the quality of the available data to characterize the hydrologic properties of the sedimentary interbeds as follows:

A-B interbed—four samples, two boreholes: "...the available samples are not adequate to hydraulically characterize the A-B interbed...A-B interbed was assigned the same hydraulic properties as the C-D interbed based on the similar lithology of the two interbeds." Vertical hydraulic conductivity varies within three orders of magnitude.

B-C interbed—six samples, five boreholes: "The samples that have been recovered are biased toward lower permeability because they are composed of finer-grained materials which are more easily recovered...the number of samples...is not adequate to hydraulically characterize the B-C interbed." Vertical hydraulic conductivity varies within six orders of magnitude.

C-D interbed—34 samples, 14 boreholes"...characterization appears adequate for the C-D interbed." The C-D interbed generally contains more clay and loam leading to better sample recovery." Vertical hydraulic conductivity ranges over seven orders of magnitude.

For the lower interbeds no samples were available.

There are potentially serious shortcomings in the assumed homogeneity of materials and flow. The interbeds in at least some places have a high degree of internal stratification and other hydraulically significant structural features (Rightmire and Lewis, 1987a; Hughes, 1993). The presence of lenses or layers of texturally contrasting materials at a vertical scale of centimeters or millimeters indicates a high likelihood that funneled flow is common in these materials. Unstable flow is also possible, and heterogeneities of the materials may cause some degree of macropore flow. Some of these preferential-flow features

may channel the bulk of water and contaminant movement within a fraction of the total volume of the interbeds. The model treats preferential flow (section 2.4.3.3) only implicitly in the inferred effective hydraulic properties of the interbeds. This treatment is similar to that for flow in the basalts, though flow in the interbeds could be complicated by the possible combination of various preferential-flow modes with nonpreferential flow.

The IRA model hypothesizes a continuous impeding layer at the top of the B-C and C-D interbeds (Magnuson and Sondrup, 1998, p. 3-7), which could represent a layer of clay at the top of these interbeds, or sediment filling of fractures in the basalts immediately above the interbed. Such feature have been described (Barraclough and others, 1976), but the main reason for including these layers is to improve the match to perched-water levels in inverse modeling for model calibration (section 6.3.2.1). At least some direct observational evidence of interbed materials contradicts this hypothesis, for example textural profiles that become generally finer with increasing depth within the interbed (Rightmire and Lewis, 1987a, p. 43; Hughes, 1993, fig. 12). Some observations support a more random distribution of clays within interbeds (Rightmire and Lewis, 1987a, p. 34). These observations strongly indicate that if such interbed-capping clay layers exist near the SDA, they are not continuous. The possible nonuniqueness of inverse modeling results could account for the better matches to hydrologic data when this hypothetical clay layer is included. Alternatively, the clay layer may serve to compensate for some other, unaccounted-for mechanism that has an impeding effect.

In a study that is being done by the USGS (K.S. Perkins and J.R. Nimmo, USGS, 1999, written commun.) to develop methodologies for drilling, coring, and characterizing the hydrologic properties of the sedimentary interbeds, continuous cores of the B-C interbed were recovered from two boreholes (UZ98-1 and UZ98-2) located southwest of the SDA (fig. 6-22). The B-C interbed at this location is approximately 10.4 m thick and has two distinct sections. The upper 5 m is composed primarily of fine to coarse sands interspersed with thin, intermittent gravel layers. The lower 5.4 m is primarily a silt loam. Nineteen core samples were used to determine the unsaturated hydrologic properties of this unit. Forty samples were used to define the unit's textural characteristics, or particle-size distribution. The clay-sized fraction in eight samples from the upper section ranges from 0 to 4 percent. The clay-sized fraction in 32 samples from the lower section ranges from 4 to 23 percent; the largest clay percentages are in samples from near the base of the B-C interbed at this location.

Saturated hydraulic conductivity of the B-C interbed at the drilled location varies within four orders of magnitude, from a minimum of 0.2 mD near the bottom of the lower section to a maximum of 3,900 mD across the entire upper section. The arithmetic average of the measured saturated hydraulic conductivity for 14 samples is 12 mD. The median value for these 14 samples from the lower section is 5 mD. Measurements of saturated hydraulic conductivity in samples from the upper section do not include the effects of the thin intermittent gravel layers, indicating that the saturated hydraulic conductivity of the upper section could be much larger than the largest value measured on the core samples.

The uppermost 0.3 m of the B-C profile at the drilled location consists of a highly oxidized, reddish, baked zone of gravelly sand overlain by massive basalt. The clay-sized fraction of this upper baked zone is approximately 1 percent.

The above example illustrates that the hydrologic properties of the composite B-C interbed at the drilled location deviate markedly from the assumption that the interbeds can be treated as homogeneous, isotropic media. Characterization of the interbeds should include definition of the vertical and lateral variability of their physical, hydrologic, and chemical properties. The validity of simplifying assumptions, which are needed to represent these geologic units in the numerical simulator, cannot be established without data that can show how these basic properties vary in space.

6.2.2.5 Aquifer properties

Controls on water movement in the SRP aquifer, as described in section 2.4.4, are assumed to be consistent with the controls on water movement in the fractured basalts in the unsaturated zone (Becker and others, 1998, p. 5-66). The flow properties of the basalts in the saturated zone, specifically permeabilities, were determined largely from aquifer test data and calibration of the saturated-zone portion of the WAG-7 model to available hydraulic head data (section 6.3.2). The basalt permeabilities determined during calibration of the WAG-10 model were initially considered in the calibration but then were disregarded because they produced a poor match to the available head data and because site-specific information was available from the aquifer tests. Potential concerns with this step of the calibration process relate to (1) the neglect of the possible effects of diversion of water from the Big Lost River (BLR) into the spreading areas (section 6.2.3.3), (2) the selective use of head data that ignored indications of transient behavior in the aquifer (section 6.2.3.3), (3) the limited head data available to specify the

boundary conditions, particularly along the western and northern boundaries of the WAG-7 model, and (4) the exclusive use of prescribed heads along the boundaries and the absence of any constraints on the ground-water flux, which could allow any model that includes permeabilities in the same ratios as those determined in the calibration to match the head data equally well.

The permeability estimates for the saturated-zone portion of the model were taken initially from the WAG-10 model (McCarthy and others, 1995). These estimates were 168,000 mD for zone 53 of the WAG-10 model, which corresponded to the northeast corner of the WAG-7 model, and 1,800,000 mD for zone 54 of the WAG-10 model, which corresponded to the remainder of the WAG-7 model domain. Because Magnuson and Sondrup (1998) were unable to reproduce the observed hydraulic heads by using a two-zone model and these permeability estimates, they created a more detailed model for the saturated zone that included three shallow zones and a fourth deep zone that represented the "I" basalt. Zone 1 was a large permeability (1,200,000 mD) region that extended from the northern model boundary southward into the southern half of the SDA. Zone 2 was a medium-permeability (16,300 mD) region that extended from the southern limit of Zone 1 to the southern model boundary, except near the SDA where, locally, a small-permeability region (153 mD, Zone 3, discussed below) was assumed to extend 1,000 m south of the SDA. The permeabilities of these three zones were the arithmetic mean permeabilities of large, medium, and small permeability zones identified by Wylie and Hubbell (1994) and Wylie (1996) based on transmissivities calculated from aquifer-test data and the open intervals of the wells (Magnuson and Sondrup, 1998, fig. 2-22). Permeabilities for individual wells in the three shallow zones ranged from 4 to 1,508,700 mD. The six-order-of-magnitude variability in the permeability measurements for individual wells seems to indicate that permeability is strongly affected by different types of volcanic deposits, fissures, and dikes. In the final calibrated model, a fourth zone representing the relatively deep "I" basalt was added to the model. Based on modeling of Rodriguez and others (1997) the "I" basalt has a permeability of 85,000 mD.

The existence of the small-permeability region of Zone 3 (153 mD) in the SRP aquifer southwest of the SDA (Becker and others, 1998, p. 5-66) is supported by data from aquifer tests from eight wells that trend northwestward along the southern boundary of the SDA. Values of effective hydraulic conductivity in these wells range from about 0.003 to 0.3 m/d and are among the smallest measured values at the INEEL. Values of hydraulic conductivity in this range are attributed by Anderson and others (1999) to concealed dikes. Dikes, if present, probably are oriented at a high angle (perpendicular) to the main direction of ground-water flow and may form local barriers to flow. As currently (1999) implemented in the IRA model, the small permeability region is assigned to the upper portion of the aquifer beneath the southern half of the SDA and affects the movement of nitrate by acting as a partial dam, that is by forcing water and dissolved nitrate in it to go around or under the small permeability region (Magnuson and Sondrup, 1998, p. 4-9). If this small permeability region is related to concealed dikes, these dikes probably extend from beneath the base of the aquifer to the top of the C-D interbed in the unsaturated zone, so that water and wastes in this area must go around or through the zone of dikes. Dikes are postulated as linear, discontinuous features in the SRP (Anderson and others, 1999). The available data strongly support the assumed small-permeability region, though its hydraulic effects are represented only approximately in the IRA model. If the actual permeability were smaller than that assumed in the model, COPC concentrations in the aquifer under the SDA likely would be greater than the model predicts.

The effective porosity of basalt probably ranges from 0.10 to 0.25 (Ackerman, 1995). Although a reasonable value of porosity of 0.05 was used for SDA flow simulations, this value is significantly less than a value of 0.21 derived from calibration of an advective transport model of the SRP aquifer system (Ackerman, 1995) and is conservative for contaminant transport.

6.2.2.6 Heterogeneity and anisotropy of hydraulic properties

The hydraulic properties within lithologic units, both basalts and interbeds, are assumed homogeneous (Becker and others, 1998, p. 5-65), as noted in section 6.2.2.1 above. The effects of this simplification are the previously mentioned omission of preferential-flow mechanisms and the impeding barrier effects that could affect contaminant transport.

Most of the subsurface is highly anisotropic (section 2.3). There are strong possibilities for small-scale (intralayer) anisotropy, for example, where basalt fractures tend to be more vertically or horizontally oriented. Large-scale (multilayer) anisotropy is a certainty, if in no other way than because a basalt-sediment interface will have markedly different effects on horizontal and vertical flow. The net large-scale anisotropy was assessed by inverse modeling during model calibration (Becker and others, 1998, p. 3-31): horizontal K exceeded vertical K by an estimated factor of 30. The magnitude of anisotropy does not have a

sound independent basis for estimation, however, which partly explains why different degrees of anisotropy have been reported by different sources (Barraclough and others 1976, p. 48; Magnuson and others, 1995). The anisotropy quantified in the IRA model is what gives the best performance of this model, but cannot be fully evaluated with respect to known properties of the subsurface.

6.2.3 Unsaturated-zone flow

6.2.3.1 Infiltration

Estimating the rates of water movement through the trenches containing the waste is essential because the likely pathway for nonvolatile contaminants to reach the underlying aquifer is dissolution by and transport with infiltrating water. These estimates were made by Martian (1995) using a computer code (UNSAT-H) and moisture profiles in the surficial sediments determined using a neutron probe at 17 shallow boreholes at the SDA. Using soil moisture data from 1994 and 1995 (Bishop, 1996), Martian (1995) first estimated the soil properties at each of the 17 boreholes and then used historical climate data in combination with the estimated soil properties to calculate daily infiltration at each borehole between 1952 and 1995. The data from 1994 and 1995 indicated that the character of the spring thaw, whether it was abrupt so as to generate runoff over partially frozen ground or slow enough to allow melting snow to infiltrate where it lay, was an important variable in determining the distribution of infiltration at the SDA. Therefore, historical information on the character of the spring thaw during 1952–95 was used to adjust the precipitation data used in the models for individual boreholes to account for the timing and amount of runoff during the spring thaw. The adjustments for individual boreholes used precipitation multipliers determined from the 1994 and 1995 calibrations, years in which the character of the spring thaw differed appreciably. Yearly infiltration rates at the 17 boreholes and detailed topographic contour maps were used to estimate spatially variable distributions of infiltration at the SDA, both temporally constant and temporally variable. The spatial average of 8.5 cm/yr was larger than the average winter precipitation of 6 cm, which Martian (1995) attributed to the drifting of snow at the SDA. In spite of the detail and thoroughness of the Martian (1995) study, significant uncertainty remains concerning infiltration at the SDA. This uncertainty arises because (1) only 2 of the 17 neutron probe access boreholes used in the calibration were located in the disturbed soils in the waste emplacement trenches (the other 15 boreholes were in the undisturbed soils between the trenches), (2) the amounts of water that infiltrated during floods in 1962, 1969, and 1982 is uncertain, and (3) only two years of data (1994–95) were available to calibrate the infiltration model. These uncertainties were acknowledged by Magnuson and Sondrup (1998, p. 6-3).

Infiltration is assumed to be spatially and temporally variable (Becker and others, 1998, p. 5-65). This assumption is surely valid qualitatively, but like the issue of variability of subsurface properties discussed above, it is not certain whether the quantification of variability incorporated into the model is adequate to make this treatment conservative. A particular concern is whether infiltration could be concentrated at certain locations over a smaller spatial scale than covered by the grid used for this purpose (Magnuson and Sondrup, 1998, p. 2-18).

6.2.3.2 Percolation

After water infiltrates, it moves in various ways through the unsaturated zone, including vertical redistribution, deep percolation, and lateral flow. All of these have potentially significant effects on the transport of COPC's

Macropore flow, deflected or funneled flow, and unstable flow may be important modes of subsurface transport, as noted in chapter 2. For the most part, these preferential-flow features are not treated explicitly in the model. Two exceptions include (1) the incorporation of areal variations in infiltration and volatile organic compound (VOC) exchange with the aquifer, and (2) the implicit inclusion of preferential flow in the effective properties of the granular media as noted above in section 6.2.2. The treatment of areal variations in infiltration and VOC exchange with the aquifer accounts for some of the preferential flow, but at a much coarser spatial resolution than that of the preferential flowpaths. To the extent that the inverse modeling that was used to determine effective properties is based on measured data that reflect the effect of preferential flow, the resulting property values could represent preferential flow in combination with non-preferential flow. These two treatments can accommodate some effects of preferential flow, but could be inadequate for addressing issues such as travel times through the unsaturated zone and the possibility that lateral flow is a significant contaminant transport process.

As an example, the age-dating study of Busenberg and others (1993) gives evidence for significant preferential transport of solutes. In this study, concentrations of chlorofluorocarbons in the saturated zone that originated during the previous 50 years were detected. Results of this study reflect transport in both preferential and nonpreferential pathways. Busenberg and others concluded that, at

the INEEL, "most ground waters have ages of 14 to 30 years." In comparison, the IRA model (Magnuson and Sondrup, 1998, p. 3-34 to 3-38) predicts travel times at the SDA of 23 to 216 years. The difference in travel times indicates that preferential flow, not accounted for by the model, could be significant. Magnuson and Sondrup (1998, p. 3-38) noted that the limitations of model discretization could be important in this sort of discrepancy.

6.2.3.3 Lateral flow

The numerical simulator for flow in the unsaturated and saturated zones at the SDA does not treat the effect of water diverted into the spreading areas from the BLR (Magnuson and Sondrup, 1998, p. 2-30). The spreading areas are approximately 1,500 to 1,600 m west and south of the SDA (fig. 6-22). These flood-control spreading basins were constructed in 1958, enlarged in 1984, and have been used intermittently since 1965 to regulate flow in the BLR (Bennett, 1990). A record of flow diversions into the spreading areas from January 1965 through January 2000 is shown in figure 6-23. Until recently, data have been lacking to demonstrate convincingly a direct connection between operation of the spreading areas and ground-water flow in the subsurface at the SDA. Some earlier investigators have inferred this connection as a possibility on the basis of limited unsaturated-zone, but substantial saturated-zone, data.

Because of the proximity of the spreading areas to the SDA and the large quantities of water that have been and could be diverted into these spreading areas, the effect of the spreading areas on flow and contaminant transport at the SDA needs to be evaluated. The validity of the conceptual model of flow and transport at the SDA will remain in question until these effects are determined.

Although the effect of the spreading areas on flow and transport at the SDA is not included in the IRA model, infiltration and recharge from the spreading areas are cited in the IRA as possible explanations, among others, to account for (1) the inability of the model to simulate perching at USGS 92 (implied in discussion of perched water, Magnuson and Sondrup, 1998, p. 6-4), (2) lower nitrate concentrations in perched water at USGS 92 (Magnuson and Sondrup, 1998, p. 4-4), and (3) the presence of carbon tetrachloride contamination in the SRP aquifer north and east of the SDA (Magnuson and Sondrup, 1998, p. 4-60).

Several earlier investigators hypothesized that water from the spreading areas could affect flow in both the unsaturated and saturated zones beneath the SDA. Barraclough and others (1976) proposed that recharge from these off-channel diversions could result in the formation of a ground-water mound beneath the spreading areas, which could cause local gradients in the aquifer to change direction temporarily in response to the assimilation of the recharge water into the regional aquifer. As depicted by Barraclough and others (1976, p. 55), the subareal extent of the mound and its effect on local gradients in the saturated zone beneath the spreading areas (fig. 6-24) is apparently large enough to cause ground water in the SRP aquifer beneath the SDA to move in a north and east direction. These gradient reversals could provide a mechanism to explain the apparently incongruous presence of carbon tetrachloride in the SRP aquifer in wells upgradient to the north and east of the SDA (M14S, M7S, and M6S).

Pittman and others (1988) mapped the rise in water levels that resulted from large volumes of water that were diverted into the spreading areas between July 1981 and July 1985 (fig. 6-23). During this four-year period, more than 9.87×10^8 m^3 of water was diverted from the BLR into the spreading areas. These diversions resulted in a net water-level rise of from 2.4 to 3 m beneath the spreading areas and from 1.8 to 2.4 m beneath the SDA (fig. 6-25). These differential head changes are much larger than local head changes that define the regional flow gradient near the SDA, and lend support to the ground-water mound hypothesis of Barraclough and others (1976).

Rightmire and Lewis (1987b) presented stable isotope data, $\delta^{18}O$ (oxygen) and $\delta^{2}H$ (deuterium), to show that perched water from USGS 92 could be derived, partly, from lateral flow of water in the unsaturated zone that infiltrates beneath the spreading areas. They hypothesized that water infiltrating beneath the spreading areas accumulates as a perched mound on the C-D interbed at a depth of 73 m and moves laterally about 1,500 m to the northeast beneath the SDA. Lateral migration of recharge water could dilute contaminated water that has infiltrated beneath the SDA. Dilution is one mechanism that could account for the smaller nitrate concentrations of perched water in well USGS 92.

Hubbel (1990) presented water-level records from USGS 92 and 88-02D as additional evidence to suggest that perched water-level recovery rates in USGS 92, and to a lesser extent in 88-02D, correlate with the historical record of inflows into the spreading areas.

The large diversions of water that occurred in the early to mid-1980's coincided with an anomalous 23-m rise in water levels in well USGS 88 (fig. 6-26). This monitoring well is completed in the SRP aquifer and is located midway between the spreading areas and the SDA (fig. 6-22). The water level in this well rose abruptly more than 23 m beginning in mid-1983 through late 1984 and did not return to pre-rise levels until late 1991. The water level in

this well has not risen comparably since the large spreading area diversions of the early to mid-1980's. The water level in this well peaked shortly after the record monthly diversion of 6.14×10^7 m^3 into the spreading areas in June 1984 (Bennett, 1990, p. 42). This rise is much greater than the regional rise near the SDA (fig. 6-23) and probably reflects filling of the well from spreading-area water that moved laterally in the unsaturated zone above the aquifer. The slow decline in water levels since the mid-1980's suggests that aquifer permeability in this area is very small.

To test some of these hypotheses, the USGS introduced a polyaromatic tracer (1,5 naphthalene disulfonate) into spreading areas A and B (fig. 6-22) in late June 1999 (Nimmo and others, 2002). The purpose of this experiment was to determine if it is possible for spreading-area water to move beneath the SDA. Monitoring results indicated that it is possible for water from the spreading areas to move laterally within the unsaturated zone beneath the SDA in a relatively short period of time. Test results also indicated that, at least locally, vertical movement of water through the unsaturated zone to the water table beneath the spreading areas is also rapid. The latter suggests that there could be significant gaps in the interbeds beneath the spreading areas or that, locally, the vertical permeability of the interbeds could be very large. The locations of the wells used to monitor tracer movement near the SDA are shown in figure 6-22.

The tracer was introduced into spreading area A on June 21, 1999, and into spreading area B on June 22 and 23, 1999 (fig. 6-22). This tracer was first detected in water from well USGS 92 on September 20, 91 days after its introduction into the spreading areas. This detection was followed by additional detections on October 21 and November 15, 1999. Analyses of two archived water samples from well USGS 92, dated March 30, 1999 and April 18, 1997, indicate that the tracer used in this experiment was not present in the perched water in this well prior to this test. The tracer was detected in SRP aquifer water in well USGS 120 only 9 days after tracer introduction. The tracer also was detected in perched water recovered from the basalt immediately above the B-C interbed in well USGS UZ98-2 (18 days after tracer introduction), in perched water recovered from the B-C interbed in well USGS UZ98-1 (65 days after tracer introduction), and in five boreholes completed in the B-C interbed at the LSIT. The LSIT boreholes were first sampled in December 1999, approximately 180 days after tracer introduction.

A critical assumption of the IRA model is that essentially all flow beneath the SDA originates as infiltration from local precipitation and runoff at the SDA. Within the SDA, modeled infiltration fluxes are spatially variable and range from 0.64 cm/yr to 24.1 cm/yr for a net infiltration rate of 8.5 cm/yr. The cumulative volume of modeled infiltration at the SDA was approximately 34,300 m^3/yr (Magnuson and Sondrup, 1998, p. 2-19). Outside the SDA, infiltration was assumed to be 1.0 cm/yr (Magnuson and Sondrup, 1998, p. 2-19). Although the amount of lateral flow in the unsaturated zone beneath the SDA from the spreading areas cannot be quantified on the basis of the tracer data, the magnitude of these potential fluxes could be a significant component of total flow in the unsaturated zone, and could be much larger than that derived from local precipitation and snowmelt. If the 2.71×10^7 m^3 of water that was diverted between May 30 and July 2, 1999 is the minimum diversion necessary to initiate lateral flow in the unsaturated zone beneath the SDA, then the spreading-area diversion record (fig 6-23) indicates that many such lateral flow events have been initiated during the past 35 years.

The tracer results and other supporting information make it difficult to ignore the possibility of spreading area effects on contaminant transport beneath the SDA. Calibration of the numerical model is based on matching simulations to (1) perched-water levels, (2) nitrate concentrations in perched water and the aquifer, and (3) carbon tetrachloride concentrations in the unsaturated zone, which in turn are based on a conceptual model that is presumed to be dominated by vertical flow through the unsaturated zone. As demonstrated by the numerical simulator for the IRA, infiltration rates at the SDA are not sufficient to sustain lateral flow in the unsaturated zone on a scale large enough to transport contaminants away from the SDA. The present formulation of the IRA model guarantees that all waterborne contaminants, whether dissolved or in suspension as colloids or macromolecules, eventually will percolate through at least one of the sedimentary interbeds beneath the SDA before reaching the aquifer; therefore, the likelihood of these contaminants bypassing the deeper C-D interbed is small, although the model formulators recognize the distinct possibility that gaps could exist in the C-D interbed beneath the SDA (Magnuson and Sondrup, 1998, p. 6-2). The inability of the numerical simulator to match perching conditions at well USGS 92, the smaller nitrate concentrations in perched water at USGS 92, and the presence of carbon tetrachloride in the SRP aquifer north and east of the SDA, are all difficult to reconcile with the current (1999) conceptualization and numerical formulation of unsaturated and saturated flow at the SDA.

The significance of spreading-area recharge on model predictions of radionuclide concentrations cannot

be quantified at this time. The detection of the introduced tracer in well USGS 92 represents a single, isolated sampling point in an extremely heterogeneous and anisotropic environment. Without additional evidence of lateral flow from other locations, it is not possible at this time to determine the extent of lateral flow beneath the SDA. The detection could be only an extreme example of channeled flow. However, the possibility of widespread lateral flow cannot be discounted given the tracer detections at the LSIT site. Few deep wells are available to sample perched water and contaminants immediately above the C-D interbed. In the 1999 tracer study, only two wells were available to access water in the unsaturated zone below the B-C interbed at the SDA. Samples of perched water were collected from both wells, but the tracer was only detected in water from well USGS 92.

Lateral flow in the unsaturated zone could facilitate contaminant transport to the SRP aquifer by intercepting waterborne contaminants that otherwise would percolate into and be adsorbed by the underlying sedimentary interbeds; however, lateral movement, by itself, does not necessarily imply a greater likelihood that waterborne contaminants will be transported to the aquifer. Dilution and dispersal of waterborne contaminants over a large area could provide greater opportunity for media sorption by (1) reducing competition for sorption sites, (2) producing changes in solution chemistry that are favorable for sorption, and (3) increasing the availability of sorption sites. However, uncertainty about the lateral continuity, elevation, thickness, and hydrologic and geochemical properties of the interbeds, and uncertainty about the quantity of underflow from the spreading areas, become limiting factors on modeling a flow system where lateral flow could be a substantial component of the total flow.

6.2.4 Contaminant input and transport

6.2.4.1 Source term

The source-term and source-term release-rate model were not evaluated by the review panel. The authors of the numerical simulator and the IRA have expressed serious reservations about the lack of a qualified calibration of the source-term release-rate model (Becker and others, 1998). The review team concurs that this is a major deficiency that is at least as important as other issues related to the formulation of the computational scheme to predict radionuclide transport and needs to be resolved before completion of the Remediation Investigation and Feasibility Study (RI/FS). A brief discussion of the source term is provided in section 2.5.1 of this report, and a review of the radionuclide sampling data at the SDA is provided in chapter 3.

6.2.4.2 Solute transport

Solute transport is described in chapters 4 and 5 of this report.

6.2.4.3 Colloid transport

Colloid transport is discussed in section 4.5 of this report.

6.2.5 Saturated-zone flow

Flow within the aquifer and interaction between the aquifer and other parts of the hydrologic system have relatively modest effects on contaminant concentrations relevant to risk assessment. Advective flow in the SRP aquifer is affected partly by aquifer thickness and porosity of the basalt flows (Ackerman, 1995). Travel time is a function of the product of thickness and porosity, and can increase or decrease with changes in thickness or porosity. As noted in section 6.2.2.5, travel time also can increase locally in small-permeability regions, such as that downgradient from the SDA. To a first approximation, COPC concentrations in the aquifer below the SDA could be directly proportional to the travel time within the aquifer, because greater travel times directly imply that in a given time interval, less water is available for dilution of contaminants.

Water movement in the SRP aquifer is assumed to be steady, and possible episodic effects of BLR diversions to the spreading areas on flow within the unsaturated zone or the aquifer near the SDA are not included in the IRA model (Becker and others, 1998, p. 5-66). It is not known whether this omission leads to negligible error in predictions related to risk assessment, as noted by Magnuson and Sondrup (1998, p. 6-4 to 6-5) and as discussed in section 6.2.3.3 of this report.

Magnuson and Sondrup (1998) stated that simulations of flow and contaminant transport at the SDA did not consider possible local reversals in head gradients near the SDA that could result from periodic recharge from the spreading areas. However, Barraclough and others (1976) suggested that these reversals could be significant through time, and could produce periodic reversals in gradients toward the northeast and east under the SDA. If these reversals take place, they might have the additional effect of dispersing wastes derived from the SDA, such as carbon tetrachloride and nitrates, toward the northeast. According to Burgess and others (1994), concentrations of carbon tetrachloride in the aquifer are largest in the area

east of the SDA. Unless these wastes are from sources upgradient of the SDA, their distributions might be better explained in WAG-7 simulations by considering possible head reversals related to transient recharge from the spreading areas.

6.3 Review of the numerical simulator

The numerical simulator incorporates the assumptions and simplifications described in section 6.2, and allows their quantitative application. Formulation of this model was an extremely complex undertaking. This review assesses the choices made in developing and calibrating the model and the utility of the model results.

6.3.1 Description of the numerical simulator

The numerical simulations described by Magnuson and Sondrup (1998) were run with the TETRAD code. TETRAD, originally developed as an oil and geothermal reservoir simulator (Vinsome and Shook, 1993), uses numerical techniques developed over several decades of experience in reservoir simulation. The principal focus of the INEEL TETRAD simulations was the fate and transport of waste material buried at the SDA (Magnuson and Sondrup, 1998). Additional focus was defined for other phenomena, such as transport of organic constituents introduced into the subsurface from waste buried at the SDA.

TETRAD is capable of simulating the movement of an arbitrary number of components, which may be distributed among the water, gas, and oil phases in either single- or dual-porosity media. Its multiphase capabilities make it usable for both saturated and unsaturated conditions. The nonlinear component conservation equations are solved iteratively, using widely used and generally accepted numerical techniques. These numerical techniques include: (1) Newton-Raphson iteration, (2) finite-differencing techniques, (3) upstream weighting schemes of various orders for the density, permeability, mole fraction, and enthalpy terms to provide numerical stability, (4) dispersion control techniques for reducing the effects of numerical dispersion, and (5) various scaling and matrix factorization methods to provide numerical stability and flexibility in mesh design and refinement.

The modification of TETRAD to consider problems of broader hydrologic application is described by Shook (1995). The modifications included (1) the incorporation of alternative fluid property packages that describe the characteristics of fluids other than oil, gas and water (for example, dense, nonaqueous-phase liquids), (2) the equilibrium distribution of components between phases, (3) alternative boundary conditions likely to exist in hydrologic problems, (4) phase-dependent, linear and nonlinear adsorption models, (5) decay and ingrowth of mother and daughter products from radioactive and other types of first-order decay, and (6) phase-dependent dispersive transport as a result of diffusion and mechanical dispersion, with the dispersion coefficient described by a tensor.

Direct testing of the TETRAD code was beyond the scope of this review. In published test problems, the simulation results compared favorably with the results of analytical solutions for a radially symmetric geothermal problem (Vinsome and Shook, 1993); and a two-dimensional test problem involving density-driven flow with advection, dispersion, adsorption, and decay (Shook, 1995). However, TETRAD does not have as long an established history as some older hydrologic simulators and does not yet have as broad a user base to expose its limitations.

TETRAD has several known limitations. Magnuson and Sondrup (1998, p. 5-19) expressed appropriate concern regarding the use of a single convergence criterion when simulating groups of contaminants that include parent and daughter constituents at widely varying concentrations. Although TETRAD includes methods to control numerical dispersion, these methods were not always used. As explained by Magnuson and Sondrup (1998, p. 4-9), the actual dispersion in the model calibration was a poorly characterized, inseparable mixture of numerical and hydrodynamic dispersion. It is not clear to what extent the extremely small simulated concentrations of contaminants in chapter 5, "Predictive transport simulations," and elsewhere, could have been affected by numerical dispersion.

Particle-tracking methods that would avoid problems of numerical dispersion associated with the advection-dispersion equation could be considered to supplement the simulations done so far. These methods would better illustrate simulated flowpaths than contour plots of concentration or saturation values (for example Magnuson and Sondrup, 1998, figs. 3-13 and 3-14).

Much research has been published on the applicability of the advection-dispersion equation with a constant dispersivity value for describing field-scale transport (for example, Neuman (1990), Gelhar and others (1992), and references listed therein). There seems to be a consensus that dispersivity increases with scale. As indicated by the voluminous body of recent work, this is an active area of research. The simulations of contaminant transport at the INEEL would not be expected to solve problems that have engaged the hydrologic profession for decades; however,

Table 6-5. Characteristics of TETRAD discretization (model grid shown in fig. 6-1)

PLAN, OR HORIZONTAL, GRID						
Resolution level	Southwest corner location		Cell dimensions (m)		Number of columns	Number of rows
	Easting (x)	Northing (y)	Δx	Δy		
0	76,270	197,875	1,000	1,000	9	9
1	80,270	202,875	250	250	12	8
2	80,520	203,375	125	125	12	8
3	80,645	203,625	62.5	62.5	20	10

the major findings and hypotheses that have grown out of this earlier work provide a context for the interpretation of simulated contaminant transport at the SDA.

Initial conditions, boundary conditions, time steps, and convergence criteria used in the TETRAD modeling were not evaluated as a part of this review.

6.3.1.1 Discretization and grid refinement

Although the fate and transport processes the model simulates may be continuous, the TETRAD code requires information to represent the model domain as horizontal and vertical grids of discrete cells. The smallest cells defined in the discretization are 62.5 by 62.5 by 0.5 m and have a volume of 1,953 m^3. These cells represent the finest resolution simulated within the model domain.

If the entire model domain were simulated at this finest resolution, then considerably more cells than the TETRAD code can address would be required. In addition, because current modeling philosophy often recognizes that relatively fine resolution is not necessary throughout the entire model domain, various levels of resolution often are used. Consequently, different levels of resolution were used in the discretization of the model domain and the finest levels of resolution were focused on the SDA.

There are four levels of resolution in the plan discretization; they are referred to as levels 0, 1, 2, and 3 and proceed from coarse to fine. Table 6-5 defines each level and its characteristics. Level 3 consists of cells that have a plan dimension of 62.5 by 62.5 m and is roughly centered about the SDA (fig. 6-1).

The vertical grid is structured to use the finest levels of resolution for certain horizons (surficial sediments and three interbeds) in the vertical cross section. The vertical discretization is less systematic than the plan discretization. Briefly, it provides 0.5- to 2-m resolution to a depth of 14 m, 2 to 4 m resolution to a depth of 80 m, and 7 to 18 m resolution to a depth of 251 m.

6.3.2 Model calibration

The numerical IRA model was calibrated in a series of steps, each of which considered different hydrologic and geochemical data sets. Many of these steps involved some form of inverse modeling (section. 6.2.2.1). These steps are intended to follow generally accepted guidelines for numerical model calibration, which were summarized for example by Hill (1998, p. 34–39). The data used in the calibration, the estimated properties, and the potential concerns associated with individual steps in the calibration process are listed in table 6-6. In the calibration process described by Magnuson and Sondrup (1998, chapters 3 and 4), few parameter values or other features of the model were altered from their initially chosen specifications. Some general comments about the IRA model calibration are appropriate:

(1) The data sets varied considerably in quality and quantity, from the fairly comprehensive, high-quality data set for CCl_4 used to calibrate the gas-phase transport properties to the limited data set for perched water that was used to help determine unsaturated-zone hydrologic properties. A related concern is the uncertainty of data for background concentrations of contaminants moving beneath the SDA from upgradient locations, including those used in the calibration.

Table 6-6. Summary and review of IRA model calibration steps, target data, and estimated properties used by Magnuson and Sondrup (1998, chapters 3 and 4)

[SDA, Subsurface Disposal Area; WAG, Waste Area Group; USGS, United States Geological Survey]

Calibration step	Target data	Estimated properties of subsurface	Comments
Adjust flow and transport properties of basalts in unsaturated zone	Transient perched-water data for SDA subsurface	Horizontal and vertical permeability; fracture porosity; longitudinal dispersivity	Poor quality and quantity of perched water data; poor match of model to perched-water data
Estimate flow properties of basalts in saturated zone	WAG-10 model results; pump-test data; potentiometric-surface data	Horizontal permeability	Selective use of hydraulic head data; limited hydraulic head data to define boundary conditions; neglect of possible effects of spreading areas; determination only of ratios of permeabilities from different units
Introduce hypothetical low-permeability clay layers	Transient perched-water data for SDA subsurface	New layers, with clay-like properties, above interbeds	Poor quality and quantity of perched water data; poor match of model to perched water data; perching phenomenon is not well understood and thus may be unsuitable for use in calibration
Predict transport properties of nonreactive, dissolved species	Nitrate concentrations in aquifer	Liquid-phase tortuosity (for diffusion); longitudinal and transverse dispersivity	Few nitrate data available for unsaturated zone beneath the SDA; uncertainty of nitrate source term at the SDA; uncertainty of background concentration of nitrate arriving from upgradient sources; poor match of nitrate data at USGS wells
Predict transport properties of contaminants that move in both gas and liquid phase	Carbon tetrachloride (CCl_4) concentrations in soil gas and vapor-extraction wells; dissolved carbon tetrachloride in perched water and ground water	Gas-phase tortuosity (for diffusion); matrix porosity of basalts; distribution coefficient for carbon tetrachloride	Source-term uncertainty; complicated factors affecting gas transport; limited perched-water data; carbon tetrachloride sources upgradient of the SDA; poor agreement between theoretical and calibrated values of gas-phase tortuosity for some geologic units; inconsistency of allowing for gas but not liquid diffusion into the matrix
Predict transport of contaminants of potential concern	Measured concentrations of contaminants in aquifer	Distribution coefficients; specific-surface areas and apertures of fractures in basalts	Source-term uncertainty; use of nondetections in calibration

(2) As noted by Magnuson and Sondrup (1998) and discussed above in section 6.2.2.1, the results of the model calibration could be nonunique in that more than one combination of parameters and boundary conditions could produce comparable matches of the model results to the measured data. Magnuson and Sondrup (1998, p. 6-6) acknowledged "...the inherent non-uniqueness of almost any hydrogeological inverse model."

(3) An underemphasized aspect of the model calibration presented by Magnuson and Sondrup (1998) is the potential effect that their selected assumptions and simplifications for flow and contaminant transport could have on the estimated properties. For example, the infiltration of BLR diversions in the spreading areas southwest of the SDA could have contributed to perched water above the C-D interbed beneath the SDA and caused temporary reversals in head gradients within the aquifer (Magnuson and Sondrup, 1998, p. 6-4 to 6-5), but this was not considered in the calibration. The neglect of the potential effect of pumping from the SDA production well upgradient from the SDA probably also has affected the estimated properties. Several contaminants detected in the aquifer that could have originated from the SDA could have migrated upgradient from the SDA. The ability of the model to approximately produce results similar to the measured data at these upgradient wells could be related more to numerical dispersion in the transport solution than to a realistic representation of actual processes. Similarly, the conceptualization of the hydrologic system and how best to represent it (for example, the representation of the basalts as equivalent to a homogeneous, anisotropic, porous-medium without matrix diffusion versus a heterogeneous, anisotropic, dual-porosity continuum with matrix diffusion) ultimately determine the choice of properties to be estimated in calibration and the final values. Even a decision as fundamental as the representation of the hydrologic system as a continuum dictates the choice of properties to be optimized and determines the degree to which isolated detections of various contaminants can be considered in the calibration or predicted by the model.

(4) Because no quantitative objective function was defined for evaluating the goodness of the calibration, the evaluation is more subjective than if such a function had been defined and used. At various steps in the calibration, the model was judged to adequately match the data, although it was not obvious that it had done so. In particular, the calibrated model results do not adequately match much of the measured data for perched water in the unsaturated zone (Magnuson and Sondrup, 1998, figs. 3-23 to 3-26) or nitrate concentrations in the aquifer (figs. 4-19 to 4-22). However, these discrepancies could be unimportant if other model features, such as the source term, have overriding importance.

(5) Another problem with the lack of a quantitative objective function is that, although sensitivity studies were conducted, no formal methodology was used to quantify sensitivity or uncertainty in the model properties or to assess the propagation of uncertainty in the properties to determine their net effect on the fate of the contaminants. It is highly desirable to evaluate these uncertainties quantitatively, so that the importance of particular properties would be more apparent.

(6) As noted by Magnuson and Sondrup (1998, p. 6-2), the transport of VOC's and dissolved contaminants were most sensitive to their respective source terms rather than to hydrogeologic processes. The source terms are themselves uncertain and sensitive to assumptions concerning inventory volumes, drum failure rates, and release rates.

6.3.2.1. Calibration for unsaturated-zone hydraulics

The review panel has serious concerns about the calibration step for unsaturated-zone flow. One is the poor match of the model to the target data, as noted in comment (4) above. Another concern is that the assumed existence of low-permeability clay layers at the top of the B-C and C-D sedimentary interbeds is not fully supported by field data. Other, possibly less serious concerns are the poor quality and limited quantity of data for perched water beneath the SDA, the fact that the much larger amounts of water contained in the saturated-zone part of the SDA model could have masked mass-balance errors in the unsaturated-zone part of the model, and that the use of a radially symmetric equivalent porous-media model is supported only by a selective use of LSIT data.

6.3.2.1.1 Perched water

Calibration of the unsaturated-zone flow component of the model is based almost exclusively on matching flow simulations to short-term observations of perched water. Magnuson and Sondrup (1998, p. 3-11) used perched-water data for four locations above the B-C interbed and four locations above the C-D interbed to calibrate the unsaturated-zone flow component. For the most part, these data are rather poor. To simulate perching, two adjustments in the input were made: (1) A 1-mD clay layer with a porosity of 0.05 was assigned to the tops of the B-C and C-D interbeds, and (2) the horizontal permeability of the basalts was decreased from 90,000 to 9,000 mD. The clay layer was justified on the basis that (1) "...at some locations, a clay layer is encountered at the top of the sedimentary interbeds," and (2) "...a reduced zone of

permeability at the top of the interbeds also could be considered to result from sediment infilling of fractures immediately above the interbed" (Magnuson and Sondrup, 1998, p. 3-7). These two adjustments were made assuming that all flow through the unsaturated zone beneath the SDA derives from local surface infiltration near the SDA.

Data to characterize perching are limited, and mechanisms that cause perching are poorly understood. Perched water and areas of large moisture content in the subsurface are present in just about every geologic setting beneath the SDA. No consistent pattern has emerged to predict where perching will or will not occur. Most observations indicate that perching occurs in the basalts at some locations that are not in direct contact with an underlying sedimentary interbed. Perching is most likely a manifestation of preferential flow in the basalts. Except at the contact of the basalts with the small permeability clay layer, the current formulation of the numerical simulator largely precludes any realistic simulation of lateral flow in the basalts. Lateral flow in the basalts and large fluxes in the unsaturated zone, derived from a combination of vertical infiltration within the SDA and a component of lateral flow from outside the SDA (section 6.2.3.3), could be necessary prerequisites for most perched water at the SDA.

Although perched water is important, its significance as an integrator of flow and contaminant transport processes in the unsaturated zone could be overemphasized. Instead of being a dominant and widespread phenomenon, perched water could exist primarily in isolation, where water accumulates locally into dead storage. In that case most flow in the unsaturated zone could move rapidly through the basalts and into the underlying sedimentary interbeds. Moisture distribution within the sedimentary interbeds, particularly the small permeability silty-loam units, could offer a much more realistic means of calibrating the unsaturated-zone flow component of the numerical simulator. To do this, knowledge of the moisture distribution within the interbeds and a much better definition of the hydrologic properties of the interbeds are needed. Use of interbed characteristics for this kind of calibration has not yet been seriously tried, most probably because the data are not available to do so.

The use of a small permeability clay layer to simulate perching may not be conservative. The assumption of a small permeability clay layer in the model forces lateral flow above the interbeds and thus distributes waterborne contaminants over a much larger area than might actually occur in the field. The net effect of this assumption is to provide greater opportunity for waterborne contaminants to come into contact with a much larger volume of contaminant-sorbing media and thus to minimize the undesireable effect that competition for sorption sites would have on contaminant transport.

6.3.2.1.2 Travel time

Unsaturated-zone travel times from the ground surface to the SRP aquifer were determined in a post-audit assessment of the calibration of the unsaturated-zone flow component of the numerical simulator. Travel time estimates were not used to calibrate the numerical simulator, but rather to determine how well simulated travel times compare with other estimates based on different calculations to estimate travel time (Burns and others, 1994—50 years; and Maheras and others, 1994—20 to 70 years). These other estimates were based on assumptions of constant infiltration rate, instantaneous travel time through the fractured basalts, average thicknesses for the sedimentary interbeds, and gravity drainage under an assumed unit hydraulic gradient.

Travel times were simulated by applying an incremental pulse of water for a simulation period of 1,000 days beginning in 1952. This incremental pulse was superimposed on the spatially variable infiltration rates used in the original calibration of the numerical simulator. Arrival times were determined by tracking the time when the peak concentration of this pulse arrived at the top of the SRP aquifer. The results indicate that travel times inside the SDA range from 23 to 216 years. Except for the 216-year travel time inside the SDA, the simulated travel times were not judged to differ significantly from previous estimates; however, this is debatable. As discussed in section 6.2.3.2, evidence from the age-dating study of Busenberg and others (1993), in which concentrations of chlorofluorocarbons originating in the atmosphere within the last 50 years were detected in ground water indicated that at the INEEL the young fraction of "...most ground waters have ages of 14 to 30 years." The review team believes that these estimates differ significantly from those simulated in the IRA model.

Travel times to the SRP aquifer are sensitive to (1) the presence or absence of sedimentary interbeds, (2) the choice of properties, particularly the unsaturated hydraulic conductivity relations, used to represent the interbeds, (3) temporal and spatial variations in infiltration rates at the ground surface, (4) thickness of the interbeds, (5) representation of the interbeds as minimally conductive, homogeneous, isotropic units (section 6.2.2.4), and (6) the use of the small permeability clay layers to simulate perching. The much longer simulated travel times, when compared with other evidence, indicates that preferential

flow not accounted for by the model could be significant. These longer travel times also are consistent with the observation presented in section 6.3.2.1.1 that the assumption of the small permeability clay layers may not be conservative. The net effect of this assumption is the greater opportunity for waterborne contaminants to come into contact with a much larger volume of contaminant sorbing media, which could be what is reflected in the longer simulated travel times.

6.3.2.2. Calibration for saturated-zone hydraulics

After testing four scenarios for flow in the saturated zone at the SDA, Magnuson and Sondrup (1998, p. 3-1 to 3-6) chose the Case 4 scenario for the final simulation runs. This scenario used four permeability regions developed from data for 16 wells at the SDA and results from WAG-3 simulations (Rodriguez and others, 1997). Interpolated October 1994 hydraulic heads for an area from the Idaho Nuclear Technology and Engineering Center (INTEC) to Big Southern Butte (fig. 1) were used for boundaries of the SDA model domain. Simulated heads from Case 4 were calibrated to these interpolated heads and measured heads from 16 wells within the model domain. Two hydrostratigraphic units were assigned to the model: (1) undifferentiated basalt and sediment representing the upper part of the aquifer, and (2) basalt-flow group I, a thick basalt unit having small permeability where it has been measured at the INTEC, representing the lower part (section 6.2.2.5). An aquifer thickness of about 76 m was used for Case 4 simulations. Possible effects of discharges from the BLR to the spreading areas on flow within the aquifer (Barraclough and others, 1976) were not considered in the model (Magnuson and Sondrup, 1998).

All basalt flows in the saturated zone initially were assigned permeabilities from WAG-10 model results for Case 1 simulations. These permeabilities were adjusted into four regions for Case 4 simulations (Magnuson and Sondrup, 1998) as described in section 6.2.2.5. Model grids representing the upper part of the aquifer were divided into three permeability regions, a northern region having a permeability of 16,300 mD, a central region having a permeability of 153 mD, and a southern region having a permeability of 1,200,000 mD. On the basis of WAG-3 model results, grids representing the lower part of the aquifer were assigned a uniform permeability of 85,000 mD. This permeability region represents the inferred presence of basalt-flow group I, which tentatively was correlated from cores at the INTEC to four deep wells at the SDA on the basis of natural-gamma and lithologic logs (Anderson and Bartholomay, 1995). The permeability region representing flow group I is the only one of the four regions that is not based on direct measurements at the SDA. Because the presence of this flow group cannot be verified by cores from the SDA, and also because the likelihood that, if present, flow group I represents a rubbly and permeable distal facies of near-vent, ponded flows at the INTEC, the justification for this permeability region is tenuous. The approximate range of hydraulic conductivity of these four permeability regions is within the range of values estimated from more than 100 aquifer tests at the INEEL (Anderson and others, 1999).

Use of interpolated October 1994 hydraulic heads for model boundaries and calibration could impart some uncertainty and bias to simulation results for the SDA. According to Magnuson and Sondrup (1998), October 1994 heads were used for the WAG-7 model because initial attempts to use the WAG-10 model boundary heads did not produce an adequate representation of water movement in the aquifer for the local-scale SDA modeling domain. Although the subsequent use of interpolated October heads improved this representation, accountability for the mass flux of water moving through the aquifer near the SDA was lost. In addition, the accuracy of any synoptic water-level map is only as good as that allowed by the number and spacing of wells available for interpretations. Although the number and spacing of wells available for this purpose is adequate at and near the SDA, it is less than desirable for outlying areas, which are critical for accurate representations of head distributions. It is desirable, therefore, to consider all available wells in interpretations. For example, USGS 13, a well southwest of the SDA that is measured only during the spring of each year, was not represented in the interpolated October 1994 heads. Use of the data for well USGS 13 significantly changes the interpolated head distribution near the Radioactive Waste Management Complex (RWMC), as shown by Bartholomay and others (1997, fig. 9).

6.3.2.3 Calibration for contaminant transport

6.3.2.3.1 Nitrate

Longitudinal and transverse dispersivity (V_L and V_T), which affect the movement of nonreactive species dissolved in the aqueous phase, were determined by using inverse modeling to match historical aquifer nitrate concentrations. Concerns with this step of the calibration process include (1) the very limited availability of nitrate data for the unsaturated zone beneath the SDA to constrain the calibration, (2) considerable uncertainty in the source term for nitrate at the SDA, (3) considerable uncertainty in the background concentration of nitrate in the ground

water because of potential nitrate sources upgradient from the SDA, (4) the poor match of the model results with measured nitrate concentrations in water from wells USGS 88 and 89, (5) the inability to distinguish the effects of dispersivity from those of the source-term release (release rate for nitrate from the source varied slowly over time), and (6) the possible augmentation, to an unknown extent, of the hydrodynamic dispersion terms by numerical dispersion in the model. These concerns are discussed in greater detail below.

Measured nitrate concentrations in the aquifer in excess of background values were presumed to reach the aquifer as a result of advection and dispersion from the SDA (Magnuson and Sondrup, 1998, p. 4-5). The quality of the nitrate data set is poor. The measured nitrate concentrations were consistently more than 50 percent larger than the selected background concentration in water from only three of eight aquifer wells, none of which are directly below the SDA, and only one significant concentration of nitrate in perched water in the unsaturated zone was reported. Although it is possible, and sometimes preferable, to use concentration data to refine model parameters for the flow properties that determine advection velocities, this was not done in this part of the calibration. Instead, velocities were calculated from the flow model calibrated to head data and the nitrate concentrations were used only to obtain estimates of the longitudinal and transverse dispersivities. This is probably the most reasonable approach given the quality of the nitrate data. The calibration process was to vary the V_L and V_T values to match historical nitrate data for four wells (Magnuson and Sondrup, 1998, fig. 4-12) and then to compare the results with those from simulations that used the same parameters to match four USGS wells (Magnuson and Sondrup, 1998, fig. 4-13). Sensitivity analyses resulted in two significant findings. First, of the four data sets used for calibration, those for M3S, an upgradient well, and M4D, a deeper downgradient well, were completely insensitive to the selected parameters and measured and simulated concentrations were equal to background concentrations. Because a wide range of parameters reproduce the measured data, these two data sets do not contribute significantly to the calibration. The second significant finding resulting from the sensitivity analyses relates to the limitations of the applicability of concentration data obtained from wells M1SA, M3S, and M10S for the purpose of model calibration. These three wells are completed near the top 25 m of the saturated zone (Magnuson and Sondrup, 1998, fig. 4-6). Any sampling of these wells could withdraw water over the entire vertical extent of the completed interval. If there was a vertical concentration gradient over the completed interval, this sampling would cause mixing of high and low concentrations in the well bore. This mixing cannot be distinguished from hydrodynamic dispersion. In fact, the zone of completion corresponds closely to a zone where large concentration gradients are simulated for the case of small values of V_L and V_T (Magnuson and Sondrup, 1998, fig. 4-16). These aquifer data could be suited only for estimating an upper bound of the dispersivities. The steep simulated gradients at a depth of 200 m also highlight a problem with the simulation approach. The selected background concentration of 700 µg/L apparently was added after the simulations were completed, and not included in initial and boundary conditions for the simulations (Magnuson and Sondrup, 1998, figs. 4-7 to 4-11 and 4-15 to 4-18 show simulated nitrate concentrations as small as 1 ug/L). Since dispersion is most sensitive to concentration gradients, it is important to include background concentrations in the simulations because inclusion would flatten the gradient, reduce the dispersive flux, and probably increase the dispersivity values required to match the data.

A second limitation of the nitrate data set is the very limited amount of nitrate data for perched water in the unsaturated zone. Magnuson and Sondrop (1998, p. 4-5) noted that only one nitrate concentration, 925 µg/L, was reported for the perched water from well USGS 92. Simulated nitrate concentrations for water from USGS 92 were not reported. Magnuson and Sondrup (1998, p. 4-4) acknowledged that the concentration at USGS 92 could have been affected by infiltration from the spreading areas, which have an unknown nitrate concentration. This represents a gap in the data, as acknowledged by Magnuson and Sondrup, but again also raises concerns about the conceptual model because the water level in USGS 92 cannot be reproduced and the nitrate concentrations at USGS 92 are suspected to be affected by dilution.

It would be highly desirable to obtain a more complete nitrate data set for wells completed in the perched zones and in the aquifer, both within and outside the SDA. These data could improve the calibration of the flow and transport models.

6.3.2.3.2 Carbon tetrachloride

A second class of contaminants that were considered in the calibration are those that are transported in both the liquid and gas phases. Because the transport parameters affecting only aqueous-phase transport already were considered in the calibration step involving the nitrate data, the parameters calibrated during this step were restricted to those affecting gas-phase transport. These parameters were gas-phase tortuosity in the unsaturated zone (I_g) and

effective matrix porosity (n_m). Gas-phase tortuosity affects the diffusion of gas in the unsaturated zone and matrix porosity of the basalts provides additional storage for the gas-phase species and thereby slows their transport. To account for matrix diffusion, a dual-porosity model, which permits gas-phase species to diffuse into the matrix, was used in this calibration step; however, the dual-porosity model apparently was not used for simulations of radionuclide transport (Magnuson and Sondrup, 1998, p. 5-71). Dissolved aqueous-phase species were assumed not to diffuse into the matrix, even in the aquifer.

The general transport behavior of VOC's was characterized by using a relatively extensive data set for gas-phase CCl_4 in soil gas and gas-extraction wells and measured aqueous-phase CCl_4 in perched water and water from the aquifer. This step of the calibration was relatively successful despite many complicating factors affecting the transport of CCl_4, including (1) air injection during drilling of the observation and extraction wells, (2) barometric pressure changes at the ground surface, and (3) pumping of gas-extraction wells. These processes were treated in a detailed and comprehensive manner in the calibration. Some of the concerns related to this step of the modeling are similar to those related to the previous calibration step: (1) the considerable source-term uncertainty for CCl_4 makes it difficult to uniquely identify the transport parameters, (2) the detection of CCl_4 in wells upgradient from the SDA implies temporary reversals in the hydraulic gradient due to the infiltration of water from the spreading areas or pumping from the SDA production well, or upgradient sources of CCl_4—factors not considered by the model, (3) data for CCl_4 in perched water is limited, (4) for some hydrogeologic units, discrepancies between the initial values for I_g, estimated theoretically from the Magnuson and Sondrop model, and the final calibrated values are sufficiently large as to cast doubt about the realism of the model, and (5) time-averaged profiles of CCl_4 in the unsaturated zone that covered a relatively transient period of CCl_4 transport were compared with model results.

6.3.2.3.3 Detected contaminants of potential concern

The final step of the calibration process assessed the predictive capabilities of the calibrated model by comparing predicted concentrations of 52 COPC's with measured concentrations in the aquifer. This step required the use of contaminant-specific K_ds either measured for the materials from the site or reported in previous studies for comparable geologic materials (chapter 5). A concern with this step is that estimates of the specific-surface areas of fractures and of fracture apertures were required to adjust the values of the K_ds to account for only partial exposure of the contaminant-bearing water to sorptive materials in parts of the model representing fractured basalts. Therefore, this step also assessed some previously uncalibrated transport parameters. Although the effects of source-term uncertainty were not examined in this step, the required modification of the initial source terms assumed in previous calibration steps suggests that source-term uncertainty for the remainder of the 52 COPC's is an unresolved issue. Alternative source terms could be expected to result in substantial differences in the simulated contaminant concentrations reported by Magnuson and Sondrup (1998). A second concern associated with this step of the calibration process is the use of nondetections and sporadic data to evaluate the predictive transport results. Data for a specific COPC were considered sporadic if the ratio of the total number of detections of that COPC to the number of wells in which the COPC was detected was five or greater (Magnuson and Sondrup, 1998, p. 5-44), that is, if most of the detections of that COPC were made in relatively few wells. If the model failed to predict the sporadic occurrences of specific COPC's, this failure was not considered a limitation of the model; rather, the fact that the model had predicted the limited transport implied by the nondetections for water from the majority of the wells was emphasized. The sporadic data could indicate, however, that preferential transport through relatively isolated pathways in the fractured basalts, which the model is unable to predict, is the predominant mode of transport.

In one instance (Becker and others, 1998, table 5-24), the simulated concentrations for ^{241}Am, ^{238}Pu, and $^{239,240}Pu$ were compared with measured concentrations in the B-C interbed. The simulated and measured concentrations of ^{241}Am agreed within an order of magnitude whereas the simulated concentrations for Pu were two to three orders of magnitude too small. These small concentrations were attributed to geochemical processes such as colloidal transport or geochemical perturbations. Although these processes could be operating, it is also possible that the continuum approach is not capable of reproducing preferential flowpaths leading to possible contamination. Another concern about these comparisons is that although some uncertainty is given for the measured concentrations, none is given for the simulated concentrations. At the small concentrations considered, even numerical truncation and rounding could be significant and should be addressed.

6.4 Model utilization

6.4.1 Sensitivity analyses

Uncertainty is inherent in subsurface flow and transport models. This is because it is impossible to fully characterize the hydrogeologic and geochemical variables that control the flow of water and transport of dissolved, reactive solutes. It is critical, therefore, that some level of uncertainty be associated with model results. Four different types of uncertainty can be identified: (1) uncertainty in the conceptual model, (2) uncertainty in the calibration parameters, (3) uncertainty in other input parameters not adjusted in calibration, and (4) numerical uncertainty. Sensitivity analyses are a sound and practical approach for addressing these four types of uncertainties and can yield two significant results. First, they can help demonstrate which processes most strongly affect transport of radionuclides, and knowledge of these processes leads to a greater intuitive understanding of the overall system. Second, they can establish some confidence levels (perhaps quantitative and formal) about the model predictions.

This section considers only the sensitivity studies conducted by Magnuson and Sondrup (1998). In most instances sensitivity analyses were conducted for the model calibration parameters only. Sensitivity analyses for evaluating the conceptual model, the uncertainty associated with other input parameters, and uncertainty associated with numerical issues are discussed in the next section. Becker and others (1998, p. 7-6) noted that the IRA is not conservative in all respects, and that sensitivity analysis would give a more precise description of the degree of conservatism.

6.4.2 Predictions

Confidence in model predictions requires a strong confidence in the adequacy of the model and also in the assumed continuation of phenomena and trends, even though they depend on factors not represented in the existing record. A quantitative, time-specific prediction is basically an extrapolation, over time, of the modeled phenomena. However, the specific, quantitative concentration of a COPC at a particular location at a specific time, such as 100 years into the future, cannot be known with confidence because (1) some of the processes that govern its transport are not understood, and (2) the calibration target data that could account indirectly for such processes are too limited in both quality and duration. Model predictions are most useful in a comparative sense in exploring sensitivities to particular site features and management options.

A major assumption is that hydrological and meteorological conditions of the last few decades are adequately representative of the future. Another is that infiltration patterns at the SDA will not change in the future (Becker and others, 1998, p. 5-65). Assumptions like these are widely used in predictive modeling, but they are not likely to be realistic or conservative. The IRA model is based on data that typically extend back about 50 years or less. Notable exceptions include the 2 years of measured water-content profiles on which the infiltration component of the model is based. Using this 50-year data base to predict 5 years into the future would require extrapolation that exceeds the available data base by 10 percent. To predict extrapolation over the 100-year period of institutional control, twice the approximate length of the record, is much more demanding. An obvious variable is the possibility of severe climatic or geological changes. Even in the absence of such changes (which are unlikely over a 100-year period to cause major deviations outside the range of normal short-term variability), there is the problem that the last 50 years have not experienced the full range of likely meteorological or hydrologic events. For example, 1,000-year floods are not represented in the available data set, but there is a 10-percent chance that one will occur during the next 100 years. Thus, the 100-year period goes well beyond the range of available information, and extrapolation is subject to considerable uncertainty because of factors not accounted for in model development or calibration.

Although the source term includes temporal variations owing to factors such as drum failure rates, a second implicit assumption in the long-term predictions is that the geochemical conditions at the source remain constant. The current conditions at the source could be somewhat reducing because of the disposal of trash, cardboard, and metal drums. If the immediate source area is reducing, then the source term could currently be limited by the low solubility of radionuclides in the reduced forms. For example, Pu(III), Pu(IV), and U(IV) are generally recognized as being generally insoluble. If the geochemical conditions at the source become more oxidizing over time as the degradable organic carbon is exhausted, these reduced radionuclides could become oxidized and relatively mobile. In such a scenario, the source term could become stronger with time because of changes in valence state, even though the drum failure rate decreases. Temporal changes in the source term also could occur because of changes in pH and P_{CO_2} as the organic substrates in the wastes are exhausted or because of climatic changes. In

summary, the many possible changes that could occur at the source over time should be included in a complete sensitivity analysis.

Uncertainties in the predictions also arise because the adopted conceptual model does not represent the actual field conditions. Sensitivity analyses need to be conducted to examine the effect of the assumed hydrologic environment on the simulated future concentrations. Simulations could be done to examine the significance of the layering, recharge from the spreading basins, variations in interbed properties, and various other factors that can contribute to preferential flow. Preferential flow is a crucial influence that currently (1999) is poorly understood in terms of how to predict when it will occur and with what quantitative effect. Layering is not adequately represented in the model, given its importance as a possible impediment to flow, or generator of lateral flow, or configuration for preferential flow by funneling and unstable flow processes. It has been suggested that the continuum approach selected cannot account for flow features such as funneling.

Section 5.7 notes that the K_d values generally are expected to be highly uncertain for several reasons, including variations in solution composition and lack of site specific data. The impact of this uncertainty has not been considered adequately.

6.5 Summary

The IRA numerical model as implemented with the TETRAD code is a basically sound application of the current available scientific understanding of subsurface transport processes, according with standards that are accepted in the geoscientific community for models used to test hypotheses and improve the understanding of a hydrogeologic system, though not necessarily adequate for all of the applications a risk assessment might demand. For a model of such broad scope, this model was developed in a relatively short time, during which the model developers made hundreds of decisions as to what data and processes to consider. Inevitably, some decisions could be improved upon, but the review team finds few deficiencies of this type. The model developers' attempt to consider as much data in their model as they did and their overall scientific judgment in developing the model are commendable.

Limitations in the model's applicability arise mainly from (1) fundamental shortcomings inherent in any predictive modeling of a highly complex system, (2) currently inadequate scientific understanding of certain important contaminant transport processes, and (3) the poor quality, small quantity, and often minimal relevance of the data available for characterization and calibration.

The model necessarily is based on an imperfect and highly simplified formulation of the subsurface environment and its processes. One aspect of this is that the degree of spatial detail is much more coarse in such a model than the scales of heterogeneity of properties and physical and chemical processes of the subsurface. For example, the smoothing of data, as by kriging, blurs potentially sharp contrasts between dissimilar subsurface features. The model developers recognized this problem and compensated for some of its most serious aspects by forced imposition of areas of zero interbed thickness in the model domain. Other phenomena, such as preferential flow in channels a few millimeters wide, cannot be easily compensated for. Another aspect is the time scale of applicability. Quantitative predictions of the future with this model are extrapolations of hydrogeologic data that typically extend back about 50 years. The future time over which useful extrapolations can be made from such a data set is shorter than the time scales relevant to the assessment of risks.

Significant limitations in the model's applicability arise out of hydrogeologic processes that are not well enough understood by the scientific community to predict effects of these processes on actinide transport. These chiefly concern flow behavior and chemical reactions in the unsaturated zone. Preferential flow is a process that significantly affects actinide transport, but it is poorly understood in terms of how to predict when it will occur and with what quantitative effect. It also is not known how to represent the layering of geologic materials in sufficient detail to evaluate the importance of layer contrasts as a possible impediment to flow, or a generator of lateral flow, or a configuration for preferential flow by funneling and unstable flow processes. The extent to which chemical interactions between contaminants and subsurface materials inhibit the spread of contamination is uncertain because science does not yet have an adequate theory of reactive chemical transport.

Few relevant direct measurements of subsurface properties, for example unsaturated hydraulic conductivity, are available for use in this model. The available COPC detections are also not useful for calibration, even though, in an ideal situation, measured COPC concentrations would be the data of most importance for calibration and testing. Therefore the model relies heavily on parameter values obtained through inverse modeling and less direct forms of calibration. Unfortunately, even the data used indirectly for calibration are sparse and, for the most part, have undemonstrative relevance to the transport of

COPC's. Among the reasons why this relevance is not yet established are (1) that the sensitivity of COPC transport to these data was not examined, and (2) that the COPC source terms are not well established.

Despite its limitations, the IRA model has considerable value for exploring the sensitivity of projected contaminant concentrations to certain critical features of the hydrogeologic system associated with the SDA, and for testing possible consequences of alternative management strategies for assessment of their relative effectiveness. One purpose to be served in sensitivity analyses is in assessing the uncertainty of model results caused by specific deficiencies in knowledge of the subsurface transport system, for example the variation in computed COPC travel times that can be ascribed to imperfect knowledge of effective interbed permeabilities. Another purpose is in evaluating the possible effects of alterations in the system, for example whether a proposed modification of the surface-runoff management system could have significant effect on travel times. Other examples include investigating the sensitivity of projected contaminant concentrations to such hydrogeologic features as (1) alteration of infiltration fluxes associated with climatic change, (2) changes in the contaminant source term, and (3) sensitivity of projected contaminant concentrations to K_d values. The small number of sensitivity analyses completed so far in part reflects the fact that the TETRAD model, being a relatively elaborate numerical simulation code, requires considerable computer time for each run. Besides the obvious alleviation of this problem that would be afforded by faster computers than those now available, the problem could be reduced through the development and use of simpler numerical models, perhaps working in one or two dimensions, for evaluating particular sensitivities.

Our review focuses on whether this model is defensible in various applications relevant to risk assessment. We consider defensibility in terms of whether a knowledgeable scientist would judge it to be either realistic or conservative with respect to risk-assessment applications. If the standard is to make quantitative predictions that scientists would recognize as either approximations or overestimations of the concentration of COPC's at a given point in space and time, this standard cannot be satisfied with existing science and therefore not with any particular model that has been created to date. The present state of knowledge could confirm that the predicted results are what is produced by an agreed-upon predictive procedure, but not that they will correspond to future reality. These remarks should not be taken to imply that the actual future COPC concentrations will necessarily exceed the predictions, but only that the uncertainty of the specific quantitative predictions is so high that the absolute numbers are not useful for deciding whether specific standards, in terms of specifying in advance the result of future measurements, will or will not be met. The model implemented with the TETRAD code meets prevailing scientific standards as an investigative tool, though its applicability does not extend to all aspects of risk assessment.

7.0 Summary and conclusions

This review of the Interim Risk Assessment (IRA) for Waste Area Group 7 (WAG-7) 13/14 Operable Unit focused on the fate and transport of selected actinides (Am, U, Np, and Pu) derived from mixed transuranic wastes buried in shallow pits and trenches at the Subsurface Disposal Area (SDA). This review was concerned only with the actinide data and geotechnical methodologies that were used in the numerical simulator to predict releases of the long-lived actinides to the accessible environment (the Snake River Plain (SRP) aquifer). This review did not include an evaluation of the source term or the source-term release-rate model, both of which add considerable uncertainty to an already complex problem.

The scope of this review included four topical areas: (1) Review of radionuclide sampling data at the Radioactive Waste Management Complex (Chapter 3), (2) Radionuclide transport processes (Chapter 4), (3) Distribution coefficients (K_ds) and their application to transport analysis (Chapter 5), and (4) Transport model analysis (Chapter 6). Each of the aforementioned chapters includes a separate summary section. Chapter 2, Conceptual model of aqueous-phase fluid flow and contaminant transport, presents background information that describes the hydrogeologic and geochemical setting of the SDA and vicinity. Chapter 2 also includes a discussion of hydrologic concepts that are considered relevant to the various review topics. The summary and conclusions presented in this chapter highlight many, but not all of the main points presented earlier. The main purpose of this chapter is to discuss the significance of the review team's findings in the context of whether or not actinide predictions can be considered to be conservative. The reader is referred to previous chapters for additional summaries that deal specifically with the topical areas covered in this review.

An implied conclusion of the IRA, as it concerns actinide transport, is that the predictions of actinide releases to the SRP aquifer are conservative. Conservative, as used in the context of the IRA, is meant to indicate that the numerical simulator predicts actinide releases that are larger than should reasonably be expected. The guiding philosophy in developing the numerical simulator was to use technically defensible estimates for the K_ds and conservative estimates of other model parameters wherever "realistic" estimates were not available. It was not the intent of the IRA to present a worst-case scenario.

In the case of the actinides and many other aqueous-phase contaminants, calibration control is poor for both the flow component and the transport component of the numerical simulator. No attempt was made, and appropriately so, to calibrate the numerical simulator to actinide detections in the field. The limited number of detections, their sporadic and seemingly random nature, and uncertainty over whether or not these detections represent dissolved-phase transport preclude their use for this purpose. The review team concurs with the principal investigators of the IRA that using these detections for calibration purposes is of limited value. However, to imply (as was done in the IRA, Becker and others, 1998, p. 5-61) that nondetections of actinides predicted by the model are consistent with field evidence can be misleading because model predictions are below minimum detection levels. Thus, it is not possible to demonstrate objectively whether or not the present numerical simulator over or underpredicts actinide releases to the SRP aquifer. The lack of calibration control for the actinides places greater importance and emphasis on demonstrating the reliability and validity of other aspects of the numerical simulator, as discussed in following paragraphs.

The numerical simulator is developed around a conceptual model that incorporates a number of assumptions. Any assessment of model predictions must consider the validity of the conceptual model that was used to guide the formulation of the numerical simulator, the reliability of calibration controls that were used to adjust input parameters and to test the model's capability to match the historical record, and the validity of other assumptions that were used to simplify the real-world problem. Data quality and completeness largely determine the confidence that can be placed in the model's predictive capability. Of necessity, subjective judgment or professional opinion was used in the present study to supplement or substitute for the lack of data. In doing so, the distinction between what falls inside the categories of conservative, realistic, or technically defensible and what falls outside is often blurred. This is particularly evident in the way that K_ds were determined and used in the numerical simulator.

All numerical models rely to some degree on the need to simplify the real-world problem. Simplification is required either to minimize computational requirements or to represent complex systems and processes at scales that are capable of integrating the effects of many smaller scale features and interactions. Simplification invariably reduces the problem to studying how temporally averaged and spatially averaged representations interact. Often,

simplification will degrade, or in some cases, eliminate opportunities to calibrate the simulator. Care is required to ensure that the transformation from the real world to the simulated world preserves the critical elements of the problem being studied and that the simplification process does not inadvertently compromise valuable calibration opportunities that would further reduce confidence in the risk estimates. This point was made in the IRA (Becker and others, 1998, p. 7-6). Loss of calibration opportunity is a trade-off that results from simplification and the use (or overuse) of conservative assumptions.

The conceptual model of flow in the unsaturated zone beneath the SDA assumes that all flow is derived from surface infiltration and runoff within the immediate vicinity of the SDA. Infiltration is spatially and temporally variable across the SDA. Water infiltrating through the shallow surficial sediments and buried waste is redistributed as it comes into contact with the underlying basalts. If the surficial sediments are not present beneath the buried wastes, then downward percolation into the underlying basalts proceeds unimpeded, without lateral redistribution. Flow into and through the basalts underlying the surficial sediments occurs primarily as vertical flow with little or no lateral redistribution within the basalts themselves. Lateral and vertical flow occurs at the contact between the basalts and underlying sedimentary interbeds. Locally, perched water may form at the contact between the basalts and underlying sedimentary interbeds if the vertical flux exceeds the downward percolation capacity of the interbeds and the horizontal permeability of the basalts. Lateral flows derived from seepage in the spreading areas or from the Big Lost River were not considered as sources of water that could contribute to flow in the unsaturated zone or to the formation of perched water.

There is considerable uncertainty over how the exclusion of lateral flow from outside the SDA affects actinide predictions. The decision to do so was based on the lack of compelling evidence (at least not until 1999) to do otherwise, and perhaps because of lack of data to determine what component of the total flux should be assigned to flow derived from outside the SDA. Exclusion of lateral flow in the unsaturated zone from outside the SDA may represent a significant departure from real-world conditions. If so, then interpretations of field data that were used to adjust input parameters to calibrate the numerical simulator or to test its predictive capability may be seriously compromised. Until the issue of lateral flow from outside the SDA is resolved, the reliability of the numerical simulator to predict the fate and transport of contaminants in the subsurface will remain controversial.

Assuming that other aspects of the current conceptual model are applicable, predictions of actinide releases, as presented in the IRA, are presumed to be conservative for the following reasons: (1) K_ds that were chosen for actinide transport were at the low end of the range of values that were available from laboratory tests or derived from the literature, (2) gaps in the interbeds and surficial sediments were included to provide preferential pathways for the migration of actinides, (3) the sorption capacity of the basalt matrix in both the unsaturated and saturated zones was assumed to be zero, (4) the thin and discontinuous interbeds located between the C-D interbed and the SRP aquifer were excluded from the numerical simulations, and (5) only the upper portion (76 m) of the total thickness of the SRP aquifer was assumed to be available for mixing and dilution of contaminants. By design, assumptions (3) and (4) are truly conservative treatments that require no additional clarification. Assumption (2) is conservative to the extent that all gaps in the interbeds, within the areal extent of the flow field that could potentially contain waterborne contaminants, are known. Assumption (5) may be conservative, but dispersion and advective mixing processes in the saturated zone are not well characterized. Laboratory- and literature-derived K_ds to support assumption (1) lack rigorous definition, may not be applicable to a chemically evolving, mixed-waste environment, and apply only to dissolved-phase transport.

The preceding assumptions constitute the primary basis for implying that predictions of actinide releases to the SRP aquifer are conservative. Additional assumptions were included in the numerical simulator to simplify the computational scheme, improve agreement with certain field observations, or accommodate data limitations. Examples of these assumptions are: (1) representation of the basalts as a homogeneous, anisotropic, equivalent porous media, (2) use of a low-permeability clay layer at the tops of the interbeds and the base of the surficial sediments to simulate perching, (3) assignment of hydrologic properties to the sedimentary interbeds on the basis of lithologic similarity and representation of the interbeds as low-permeability, homogeneous, isotropic units, all with nearly identical hydrologic properties, (4) use of laboratory-derived K_ds that are based on tests that do not consider how the actinides may behave in the field in the presence of other mixed wastes, and (5) use of K_ds that presume that the capacity of the media to sorb contaminants is infinite, that sorption characteristics of the media are constant, and that there is no competition for sorption sites from other contaminants that may be present.

The effects of these additional assumptions on actinide predictions are difficult to assess. Assumptions based on incomplete data or lack of data are difficult to defend and are particularly vulnerable to criticism. As a minimum, these assumptions point out the lack of rigor attendant to various aspects of the present study. Assumptions (4) and (5) fall into this category. The validity of the other assumptions and their effect on actinide predictions depend on the quality and completeness of the supporting data and on how these and other assumptions were implemented and subsequently evaluated in the numerical simulator. Sensitivity analyses normally are used to evaluate the significance of assumptions on model predictions; however, these analyses were not included in the present version of the IRA and supporting documentation. Nevertheless, a qualitative critique of these secondary assumptions and their effect on the numerical simulator is presented.

(1) Representation of the hydrologic properties of the basalts—Flow in the basalts is very complex. The representation of the basalts as an equivalent, homogeneous, anisotropic, porous media largely precludes realistic simulations of preferential flow within these units. This is a tradeoff resulting from the need to simplify. Results from inverse modeling of data from the Large-Scale Infiltration Test were used to determine equivalent porous-media properties for the basalts to represent the large-scale anisotropy and heterogeneity of these units in a manner appropriate for use in the numerical simulator. This approach is a commonly used and accepted practice, even though nonunique solutions are possible. For modeling purposes, anisotropy of the basalts is represented by a 30:1 (reduced from 300:1 to simulate perching) contrast between horizontal and vertical permeability. Homogeneity of the basalts is embodied in the representation of these units as a low-porosity, high-permeability equivalent porous media. In reality, these flow units are extremely heterogeneous and anisotropic. It is highly unlikely that the true permeability distribution of the basalt flows will ever be known at a scale that would be appropriate for use in the numerical simulator to predict precisely where actinides will migrate. For purposes of the IRA, this may not be necessary if other means (discussed later under topic (3)—hydrologic properties of the sedimentary interbeds) are available to determine the cumulative effect of preferential flow in the basalts. The present modeling effort suggests that the movement of waterborne contaminants in the unsaturated zone will be confined to a relatively small area that lies beneath the immediate vicinity of the SDA. Thus, it is assumed that all contaminants eventually will contact one or more of the primary sedimentary interbeds beneath the SDA before arriving at the SRP aquifer. This hypothesis needs to be tested. Noteworthy from the perspective of conservatism, the numerical simulator does not assign any capacity to the basalt matrix to sorb contaminants in the unsaturated and saturated zones. This is a conservative assumption that should result in overpredicting actinide releases.

(2) Simulation of perched water—Calibration of the unsaturated-flow component of the numerical simulator relies almost exclusively on simulating perching that has been observed at various locations beneath the SDA. The presence of perched water is appealing because these sites offer an opportunity to sample for waterborne contaminants. The assumption is made that perching mechanisms tend to integrate the flow and contaminant transport history to the point where the perched-water body is formed. To some extent this is true, but if other sources of water outside the contributing area of the SDA are present, then the interpretation of sampling results can be misleading. Lateral flow from outside the boundaries of the SDA may lead to underestimates of contaminant releases because of dilution, dispersion, and facilitated transport of waterborne contaminants that are derived from infiltration within the SDA.

Data to characterize perching phenomena are limited and the mechanisms that lead to perching are poorly understood. Perched water and areas of elevated moisture content in the subsurface have been encountered in almost every geologic setting beneath the SDA. No consistent pattern has emerged to predict where perching will or will not occur. The sedimentary interbeds are presumed to play a major role in this process; however, most observations indicate that perching occurs in the basalts at locations that are not in direct contact with the underlying sedimentary interbeds. The inclusion of a low-permeability clay layer at the tops of the major sedimentary interbeds and at the base of the surficial sediments was needed to simulate perching and redistribute vertical flow. These adjustments were made assuming that all flow through the unsaturated zone beneath the SDA is derived from surface infiltration at the SDA. As mentioned previously, lateral flow from the spreading areas or from seepage in the Big Lost River was not considered as a source of water that could account for the local accumulation of perched water. Larger fluxes in the unsaturated zone, derived perhaps from outside the vicinity of the SDA, may be a necessary prerequisite for most perched-water occurrences.

Although perching is important, its significance as an integrator of flow and contaminant transport processes in

the unsaturated zone may be overemphasized. A different perspective of perching might suggest that it simply reflects isolated areas where water accumulates locally into dead storage and that most flow in the unsaturated zone actually moves rapidly through the basalts and into the underlying sedimentary interbeds.

The use of a low-permeability clay layer to simulate perching may not be conservative. The low-permeability clay layer forces lateral flow to occur above the interbeds and thus distributes waterborne contaminants over a much larger area than might actually occur in the field. The net effect of this assumption is to provide greater opportunity for waterborne contaminants to come into contact with a much larger volume of contaminant-sorbing media, thus minimizing the deleterious effect that competition for sorption sites would have on contaminant transport. The assumption, as implemented, presumes that there are no known gaps in the C-D interbed in the immediate vicinity of the SDA to facilitate rapid transport to the SRP aquifer. Care must be taken not to overinterpret the significance of perched water in deference to other possibilities that are less obvious but may be more meaningful for characterizing flow in the unsaturated zone.

(3) Hydrologic properties of the sedimentary interbeds—Numerical simulations indicate that the downward flux of water beneath the SDA is not uniformly distributed. This is indicated by the lateral and vertical variability in simulated water saturations within individual interbeds and between interbeds. This is a realistic portrayal of moisture distribution in the unsaturated zone. Moisture distribution patterns that are predicted by the numerical simulator are a consequence of (1) variations in the spatial and temporal distribution of infiltration at the ground surface, (2) differences in the vertical and horizontal permeability assigned to the basalts, (3) contrasts in permeability between the basalts, the interbeds, and clay layers used to simulate perching, and (4) geometric variations in the elevation, attitude, thickness, and continuity of the modeled units, particularly the interbeds. Unfortunately, there are few data to determine how well these simulated moisture distributions represent actual field conditions.

Moisture distribution within the sedimentary interbeds, particularly the low-permeability, silty-loam units, may offer the best opportunity to calibrate the unsaturated-zone flow component of the numerical simulator. As a minimum, moisture distribution within these units may provide the information needed to determine whether flux in the unsaturated zone is derived exclusively from infiltration at the SDA, or if it includes an outside component that needs to be addressed in the numerical simulations. To do this, realistic representation of the hydrologic properties of the interbeds is needed to avoid compromising the calibration opportunity afforded by this approach. The use of the interbeds in this manner has not yet been explored or exploited to its full potential; most probably because the data are not available to do so. Flux across these units can be estimated if ambient saturations and the moisture characteristic curves for these units are known.

Temporal and spatial variations in the saturation of the sedimentary interbeds can be estimated either from *in situ* measurements of matric potential, borehole measurements using properly calibrated neutron-activation probes, or laboratory measurements of core. All these methods complement each other and should be considered together. Core measurements of the hydrologic properties and ambient moisture content of the sedimentary interbeds, particularly the silty-loam units, are especially desirable.

(4) Applicability of laboratory-derived Kds—One of the major assumptions used to defend actinide predictions as conservative is derived from the fact that the K_ds used in the numerical simulator were chosen from the low end of the range of laboratory- and literature-derived values. The intent of this decision is clear; however, the quality and completeness of the available data are insufficient to demonstrate that the K_ds were selected from a representative population of test results that are reasonably representative of the site and the influence of a chemically evolving, mixed-waste environment. The K_ds used for Am, U, and Pu transport were derived from a limited number of batch tests of a single, composite, sedimentary interbed sample. This sample was prepared from a mixture of five samples with different physical and chemical properties. Forty percent of the bulk sample (the coarse fraction) was eliminated from the batch tests, possibly biasing the results toward higher K_ds because of the greater surface area represented by the finer size fraction. Furthermore, the batch tests were conducted using synthetic water containing concentrations of major cations and anions that were generally smaller than those measured in ground water and perched water near the SDA. The lower ionic strength of the solution reduces competition for available sorbing sites and leads to larger K_d estimates. The synthetic water also was undersaturated with respect to calcite, even though calcite is a common mineral phase in the sedimentary interbeds. This is a potentially serious departure from actual field conditions, because aqueous stability and mobility of the actinides may be enhanced by the formation of weakly-sorbing carbonate complexes.

The importance of carbonate complexation is demonstrated in the thermodynamic modeling that was conducted as part of this review. Formation of carbonate complexes also was suggested, along with colloidal transport, as possible explanations for the early elution of a "fast fraction" that was observed in the column experiments for Am and Pu referenced in this review.

Although the K_ds used in the numerical simulator were selected from the lower end of the range of these laboratory-derived measurements, it is not obvious that the limited data and experimental protocols provide adequate opportunity to demonstrate that these K_ds are reasonably conservative or technically defensible.

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Appendix

SIGNIFICANT ISSUES TO BE RESOLVED TO SUPPORT

AND DEFEND THE INTERIM RISK ASSESSMENT

AND ADDITIONAL WORK REQUIRED TO

RESOLVE THOSE ISSUES

Prepared by the U.S. Geological Survey

In fulfillment of Task 5 requirements of the

INDEPENDENT TECHNICAL REVIEW

OF THE INTERIM RISK ASSESSMENT

RADIOACTIVE WASTE MANAGEMENT COMPLEX

WAG 7-13/14 OPERABLE UNITS

October 15, 1998

CONTENTS

SIGNIFICANT ISSUES TO BE RESOLVED TO SUPPORT AND DEFEND THE IRA, AND ADDITIONAL WORK REQUIRED TO RESOLVE THOSE ISSUES, RWMC WAG 7-13/14 OPERABLE UNIT

By Joseph P. Rousseau, Brennon R. Orr, and LeRoy L. Knobel

I. Introduction

Background. The IRA and Contaminant Screening for the WAG-7 RI/FS (Becker and others, 1998) was prepared for the DOE by LMITCO in support of the WAG-7 comprehensive RI/FS. The purpose of the IRA was to preserve a formal record of work completed in support of the RI/FS. The draft Addendum to the Work Plan for the WAG-7-13/14 Operable Unit Comprehensive RI/FS (DOE, 1998) defined revised strategies and additional requirements for conducting the WAG-7 comprehensive RI/FS. These two reports and supporting documents will be used in completion of the draft ROD for remediation of WAG-7 by December 2002. The DOE, in order to prepare for ROD negotiations with the EPA and the State of Idaho, requested that the USGS conduct an independent technical review of the IRA, the Addendum, and associated documents.

Purpose and Scope. Modification A005 to Contract Number DE-A107-97ID13556 between the DOE and USGS, dated July 16, 1998, established additional work to be accomplished by the USGS in support of the independent technical review, as requested by the DOE. Five tasks were identified in the proposal for work. Task 1 provides a review of radionuclide data supporting the IRA, Task 2 discusses radionuclide transport processes pertinent to the Subsurface Disposal Area (SDA), Task 3 addresses K_ds and their application to transport analysis, and Task 4 discusses transport model analysis. These tasks, to be completed by July 15, 1999, will provide a detailed review of primary and secondary documents associated with the IRA.

Task 5 (deliverable report to be provided to the DOE by October 15, 1998) of this technical review is intended to provide timely interim guidance to several questions. First, what are the most significant issues that need to be resolved to support and defend the IRA? Second, what additional work is immediately required to resolve those issues? This interim guidance is offered to provide sufficient lead time to resolve those issues within the timeframe of the draft ROD (2002).

As part of Task 5, preliminary reviews were conducted of the IRA (Becker and others, 1998), results of the LSIT (Wood and Norrell, 1996), K_ds and contaminant solubilities for the WAG-7 Baseline Risk Assessment (Dicke, 1997), and the flow and transport model (Magnuson and Sondrup, 1998). Additionally, planned work elements were evaluated that were identified in the Addendum to the Work Plan (DOE/ID, March 1998). This review focused primarily on data needs rather than on analytical approaches.

II. Review of Additional Work from the Addendum that is Related to Hydrologic Transport of Contaminants

Data quality objectives (DQOs) listed in the Addendum (DOE, 1998, table 3-3) evaluated activities needed to satisfy 1996 workplan data gaps. The USGS evaluated only those DQOs that pertain to hydrologic transport of contaminants as highlighted in italics. Data gaps identified in the Addendum are summarized after each DQO.

Identify distributions of interbed soil contaminants in the unsaturated zone to help determine whether contaminants in the aquifer are derived from the SDA or an upgradient source. This DQO was to be accomplished by analyzing for contaminants in spatially distributed samples from the A-B, B-C, and C-D interbeds. This DQO was not satisfied because interbed sample results were inadequate. Pu geochemistry experiments were inconclusive and additional experiments have been defined. No determination was made about spurious detections of actinides in the C-D interbed. Perched-water monitoring continues to evaluate migration. Additional interbed sampling is not planned.

Identify distributions of water contaminants in the unsaturated zone to help determine whether contaminants in the aquifer are derived from the SDA or an upgradient source. Monitoring work is in progress. The contractor is planning to expand the monitoring network with lysimeters near soil vaults and in waste zones.

Identify contaminant concentrations in the aquifer to help determine whether contaminants in the aquifer are derived from the SDA or an upgradient source. Determination of contaminant source using analyses of ^{3}H and NO_3 plumes proved to be inconclusive. Data were inadequate to calibrate IRA models or to differentiate upgradient sources of contaminants.

Data gaps that warrant further data collection and research were identified from analysis of these DQOs. Planned work elements to meet the need for additional data were summarized in table 3-4 of the Addendum. Work elements listed in table 3-4 that pertain to hydrologic transport of contaminants and our assessment of the adequacy of these elements to fill data gaps are summarized as follows.

Perched-water and soil-moisture monitoring data (sections 4.3.7, and 4.1.4). These data focused primarily on the surficial sediments and called for quarterly monitoring of unsaturated-zone soil water and perched water over an extended time.

Continued perched-water monitoring is appropriate, as are additional experiments to define the presence of actinides in the B-C interbed. The emphasis in the Addendum appears to be on perched water within the surficial sediments. This work certainly is important, provides a better understanding of the contaminant source term, and should be continued.

In addition, deeper interbed sampling and installation of appropriately designed lysimeters are needed, not only to differentiate contaminant sources, but also to assess the role of the interbeds in the transport of contaminants. Historically, much of the deeper sampling within the boundary of the SDA has taken place from well USGS 92. The limited areal sampling is not adequate to describe the distribution of radioactive and organic chemical contaminants in water in the vadose zone, both inside and outside the SDA. Additional sampling points may become available if a corehole-drilling program is undertaken as proposed in section IV of this report. Coreholes constructed as part of the proposed drilling program could be instrumented to expand the present monitoring network.

Installation of instruments to collect leachate, vapor concentrations, and moisture measurements (section 4.3.8) and installation of lysimeters near soil vaults (section 4.3.9). Additional suction lysimeters with appropriate backfill material to collect water samples, tensiometers to monitor infiltration rates, and time-domain reflectometry waveguides to measure soil-moisture content will be installed in new shallow coreholes and drill holes.

This work again is focused solely on the surficial sediments and will provide valuable information concerning contaminant transport. However, the limited capability to collect water samples from underlying interbeds or to measure moisture content and infiltration within interbeds precludes assessment of the role of these interbeds in vertical or lateral transport of contaminants. Additional sampling points may become available if a corehole drilling program

is undertaken as proposed in section IV of this report. Coreholes constructed as part of this proposed program could be instrumented to assist in determining the extent of contaminant migration in the unsaturated zone.

Installation of upgradient aquifer-monitoring wells (sections 4.3.10, 4.4.1). Installation of five additional upgradient, aquifer-monitoring wells was planned to identify contaminant concentrations in the aquifer, to delineate the upgradient areal extent of the CCl_4 plume in the unsaturated zone, to define background water chemistry by long-term monitoring, to provide data for calibration of fate and transport models, and to differentiate between contaminant sources.

Inconclusive analyses of ^3H and NO_3 plumes clearly illustrated the need for additional upgradient wells completed in the SRP aquifer. Four of these wells have been constructed by LMITCO and have been included in the WAG-7 monitoring programs. A fifth well is planned by the USGS in FY 1999. These wells will provide valuable upgradient water-level and water-chemistry data. We strongly endorse the implementation of this work element. The process used to locate these wells was technically sound and was designed to provide the information identified by the data gap analysis. We encourage continued monitoring of these wells to provide information to better differentiate between contaminant sources.

Actinide migration mechanisms (section 4.4.5). Work elements include peer review of actinide K_d data by qualified experts, inventory of U and Pu species in samples sent to the INEEL, modeling of transport mechanisms, modeling of actinide speciation, column tests, replication of previous colloid transport work, experiments to determine adsorption of actinide complexes onto colloids, and confirmation of the effects of Pu oxidation states on transport.

The work elements identified in the Addendum to examine actinide migration mechanisms need to be accomplished. We believe that successful completion of these elements is dependent on detailed determination of bulk and clay lithology and mineralogy in the sedimentary interbeds underlying the SDA. Intact samples from proposed corehole drilling may provide additional opportunity to conduct K_d analyses that are more representative of the deeper interbeds.

III. Significant Issues Not Identified or Emphasized in the Addendum

Hydraulic and Geochemical Characterization of the Sedimentary Interbeds. We believe that the hydraulic and geochemical properties of the sedimentary interbeds are not adequately characterized to meet the needs of a comprehensive risk assessment for radionuclide migration. Only a limited number of samples were available from the A-B, B-C, and C-D interbeds to characterize the hydraulic and geochemical properties of these units. Investigators, involved in the development and calibration of a predictive simulator for the transport of contaminants in the subsurface at the SDA (Magnuson and Sondrup, 1998, p. 6-5), also have acknowledged the lack of adequate data. Considerable, and perhaps undue, reliance has been placed on a few measurements and qualitative observations to describe the hydrogeologic properties of all the sedimentary interbeds in the WAG-7 model domain, both within and outside the SDA. The extent and reliability of these data as reported by Magnuson and Sondrup (1998, p. 6-5) and McCarthy and McElroy (1995, table 3.2.1-3) are summarized as follows:

Surficial sediments – 350 samples from both disturbed and undisturbed locations: "...characterization is of high quality and shows that there is substantial spatial variability in hydraulic properties..." Vertical hydraulic conductivity varies over four orders of magnitude (McCarthy and McElroy, 1995, p. 3-13).

A-B interbed – 4 samples, 2 boreholes: "...available samples are not adequate to hydraulically characterize the A-B interbed." "...A-B interbed was assigned the same hydraulic properties as the C-D interbed based on the similar lithology of the two interbeds." Vertical hydraulic conductivity varies over three orders of magnitude.

B-C interbed – 6 samples, 5 boreholes: "...number of samples...not adequate to hydraulically characterize the B-C interbed." "The samples that have been recovered are biased toward lower permeability because they are composed of finer-grained materials which are more easily recovered." Vertical hydraulic conductivity varies over six orders of magnitude.

C-D interbed – 34 samples, 14 boreholes: "...characterization appears adequate for the C-D interbed." "The C-D interbed generally contains more clay and loam leading to better sample recovery." Vertical hydraulic conductivity varies over seven orders of magnitude.

Lower interbeds – no samples.

The lack of adequate hydraulic data for the sedimentary interbeds within the SDA is due in large part to difficulty in obtaining complete core samples from these loosely consolidated units. Geochemical and lithologic data for the sedimentary interbeds are inadequate for the same reason. Outside the SDA, borehole coverage is extremely limited as well, and definition of the hydraulic and geochemical properties and of the generalized stratigraphy of these units is practically nonexistent.

Within the immediate vicinity of the SDA, the composite thickness, elevations, and orientations of the individual interbeds are, for the most part, well defined. Minor exceptions may be present, particularly in areas of the SDA where borehole coverage is limited (Magnuson and Sondrup, 1998, p. 6-2). Outside the SDA, definition of the sedimentary interbed stratigraphy is based only on a few widely spaced boreholes, and implications on subsurface flow and transport modeling at the SDA are uncertain.

Understanding the role of the sedimentary interbeds in retarding the migration of radionuclides from the SDA to the SRP aquifer requires much more rigorous definition of the hydraulic and geochemical properties of these units than is currently available. The interbeds, at best, are imperfect hydrologic barriers. In general, rapid downward movement of water through the fractured basalts in the unsaturated zone is retarded at interbed boundaries or above sediment- or precipitate-filled fractures near the base of the basalts that are in contact with these interbeds. This process was observed and documented in the controlled, Large Scale Infiltration Test (LSIT) south of the SDA (Wood and Norrell, 1998). Most of the flow through the unsaturated zone is in fractures and narrow, preferential channels in the basalt. This preferential flow can transport contaminants much faster than more uniform piston flow can. Interbeds may be a major retarding influence if they act to spread out and homogenize the preferential flow that enters from the basalt fractures. Alternatively, they may have little effect if flow locally is channeled and directed over or around the layer boundaries until a breach in the vertical flow barrier is encountered.

The contaminant retardation efficiency of the sedimentary interbeds depends largely on the flux within and across these units and on the cation exchange capacity (CECs) of these units. Maximum retardation efficiency is achieved if flow occurs through the sedimentary interbeds. During periods of high infiltration, lateral flow above the sedimentary interbeds may be a significant component of the total flow, and contaminant retardation efficiency may be much less than might otherwise prevail because flow would occur primarily in the basalts. This aspect of the role of the sedimentary interbeds on radionuclide migration in the unsaturated zone has not been adequately addressed, perhaps because of the lack of sufficient data with which to generate meaningful simulations.

The current predictive simulator for subsurface pathway on contaminant fate and transport does not include the possible effects of episodic infiltration in the spreading areas on contaminant transport at the SDA (Magnuson and Sondrup, 1998, p. 2-30). Rightmire and Lewis (1987) documented the possibility of significant lateral flow in the unsaturated zone beneath the SDA from infiltration of Big Lost River (BLR) diversions into the spreading areas south and west of the SDA. In this earlier study of the hydrogeology and geochemistry of the unsaturated zone at the SDA, perched water samples that were collected from above the C-D interbed at USGS 92 were shown to be depleted in the stable isotopes deuterium and ^{18}O, suggesting that this water was derived from recharge in the spreading areas and not from vertical infiltration in the SDA. In contrast, the stable isotopic signatures from perched water above the shallower B-C interbed

in well 77-2 at the SDA indicated an evaporative influence, suggesting that the source was infiltration of local meteoric water. Furthermore, the historical record of perched-water levels in USGS 92, dating back to 1972, correlates remarkably well with the records of BLR diversions into the spreading areas (Joel Hubbell, LMITCO, oral commun., 1998). Lateral flow in the unsaturated zone, possibly originating from episodic recharge in the spreading areas, also may be responsible for the observed CCl_4 plume in the SRP aquifer north and east of the SDA.

The manner in which water moves within, on, and through the sedimentary interbeds in transit to the SRP aquifer may: (1) accelerate or retard contaminant transport, (2) concentrate or dilute contaminants, and (3) determine whether flow primarily is vertical or horizontal. It is therefore important that sufficient data be made available so that critical simplifying assumptions, needed for the final formulation of the predictive simulator for subsurface pathway, can be adequately defended.

A corehole drilling program to provide better and more defensible definition of the role of the sedimentary interbeds in contaminant migration processes at the SDA is presented in section IV. The drilling of these coreholes will also provide additional opportunities to help satisfy some of the DQOs identified in the Addendum as discussed in section II. Additionally, the proposed drilling program will provide a unique opportunity to expand on the Rightmire and Lewis (1987) study of the hydrogeology and geochemistry of the unsaturated zone at the SDA.

Laboratory Performance and DQOs. The sporadic detections of contaminants at some sample sites, many of which are at the method detection limit, combined with the fact that detections frequently are unconfirmed by quality assurance samples, indicate that problems may be associated with sample collection methods, sample handling in the laboratory, analytical methods, processing of raw analytical data, or reporting of analytical results. In addition, the previous use of more than one laboratory creates difficulty in comparing detections near the method detection limit. Resolution of these data discrepancies is critical to understanding the movement of contaminants in the unsaturated zone. Examples of problematic data follow (uncertainties are reported as one estimated sample standard deviation; units are in picocuries per liter)

Well	Date	Laboratory	Radionuclide	Sample type	Concentration
M4D	Nov 1993	Barringer	Pu-239, -240	Filtered	ND
				Duplicate, F	1.3±.3
				Unfiltered	ND
				Duplicate, U	ND
[Problem—Inability to reproduce a result that was well above the analytical method detection limit]					
M3S	Oct 1997	EPI	Am-241	Unfiltered	.04±.01
				Reanalysis.	02±.02
[Problem—Reporting results less than the analytical method detection limit as positive results]					
M1S	May 1998	EPI	Am-241	Primary	2.0±.1
		EPI		Replicate-split	ND
		EPI		Replicate-split	ND
		Paragon		Replicate-split	04±.02
		Paragon		Replicate-split	003±.011
		OS lab		Co-sample	<0.05

[Problem—Inability of the same lab and other labs to reproduce a result that was well above the analytical method detection limit]

IV. Recommendations for Additional Work to Resolve Significant Issues

Two specific programs are recommended to resolve significant issues identified in section III. These consist of a comprehensive, integrated corehole-drilling program and a laboratory technical review.

Corehole-drilling and testing program.—The hydraulic and geochemical properties of sedimentary interbeds beneath the SDA have not been adequately addressed in the IRA, Addendum, and ancillary documentation. A comprehensive, integrated corehole-drilling program is needed to resolve issues related to the transport of contaminants

through the unsaturated zone and the effect of episodic recharge in the spreading areas on lateral movement of water in the unsaturated zone. Two key assumptions are essential to the successful execution of the recommended program: (1) The corehole-drilling program will provide complete, relatively undisturbed cores from the land surface through the C-D interbed at many widely dispersed sites within the WAG-7 model domain, and (2) if perched water is encountered during drilling operations, representative water samples will be immediately collected for chemical, isotopic, and contaminant analyses, particularly in the vicinity of the RWMC.

Techniques for obtaining relatively undisturbed core from unconsolidated sediments presently are being developed. These techniques can provide the samples needed to characterize hydraulic and geochemical properties of the A-B, B-C, and C-D interbeds. The inability to obtain these samples has been a major shortcoming of previous drilling efforts.

Scope

The scope of a corehole-drilling program needed to adequately characterize the hydraulic and geochemical properties of the sedimentary interbeds includes the following work elements.

-Approximately 24 to 36 coreholes will be dry-core drilled to collect core (hole size approximately 13 cm) from the land surface through the C-D interbed, with an average depth of approximately 90 m. These coreholes will be located to best sample the interbeds within the WAG-7 model domain, to include sites that will provide information at the SDA, between the SDA and the spreading areas, and to the northeast where contaminants have been detected in the unsaturated zone and aquifer. Corehole-drilling operations will include reaming of the corehole after coring through the B-C interbed and installation of steel casing across the B-C interbed to advance the corehole to the target depth.

-Sedimentary interbed core will be recovered and preserved in Lexan[4] liners.

-Perched water will be sampled immediately when encountered during drilling operations.

-Geophysical logs will be run in each corehole; log suites will include gamma, neutron, and density logs.

-Video logs will be run in each corehole.

-Each corehole will be prepared for followup monitoring, instrumentation, abandonment, and future deepening to support additional work needed to meet DQOs identified in section II.

-Hydraulic testing and geochemical analyses will be conducted on recovered cores, particularly those of the sedimentary interbeds and the basalt-interbed contacts. Laboratory tests of interbed core samples will provide spatial and vertical characterization of hydraulic and hydrochemical properties of the A-B, B-C, and C-D interbeds. These properties are needed to evaluate contaminant transport through the interbeds, potential for lateral flow from the spreading areas, and lateral migration of contaminants to the northeast of the SDA. Laboratory tests ofthe hydraulic properties of interbed cores should include detailed profiles of grain size, permeability, and water content. Laboratory tests of hydrochemical properties should include detailed profiles of the interbed mineralogy and interstitial water chemistry. The interbed mineralogy should include a detailed breakdown of the clay minerals present and their relative proportions. In addition, interbed samples could be used to satisfy DQOs calling for further tests for K_ds and actinide transport as noted in section II of this report.

[4]Use of brand names does not constitute endorsement by the USGS

Objectives

Implementation of this integrated corehole-drilling program will achieve the following objectives and can be completed in sufficient time to meet milestone dates associated with the WAG-7 ROD.

-Better definition of perching and lateral flow mechanisms within the basalt and sedimentary interbeds.

-Importance of episodic recharge from the spreading areas relative to contaminant transport in the unsaturated zone at the SDA.

-Better definition of the hydraulic properties of the sedimentary interbeds and the basalt/interbed contacts. These properties include permeability, porosity, and moisture content.

-Better resolution of the spatial continuity, thickness, and orientation of sedimentary interbeds within the WAG-7 model domain.

-Definition of the clay mineralogy within each interbed.

-Development of a defensible methodology to assign representative cation-exchange capacities to the sedimentary interbeds.

Laboratory Technical Review and DQOs. —The use of more than one laboratory for radiochemical analytical work that supports the ROD for remediation of WAG-7 is undesirable and makes comparison of data difficult. Review of past laboratory technical procedures to eliminate historical spurious radiochemical data is not feasible. A technical review is needed to eliminate future uncertainty over the reliability of laboratory analytical procedures. A consistent means of reporting data also needs to be established.

-A single laboratory should be selected to analyze all the data under a consistent set of DQOs. The selected laboratory should be contracted for the duration of the data collection process and should be audited on a routine basis.

-An independent audit of the selected laboratory should be conducted prior to awarding the contract. The preselection audit should be jointly conducted by independent parties such as DOE, USGS, INEEL Oversight Committee, and EPA. The audit should be conducted under the auspices of the guidelines contained in "Manual for the Certification of Laboratories Analyzing Drinking Water. Criteria and Procedures. Quality Assurance. Third Edition, April 1990. EPA/570/9-90/008."

-The audit should include an on-site visit, and the selected laboratory should participate in appropriate round-robin programs such as those conducted by EPA and DOE (RESL).

-For reporting low-level data, we recommend that the approach that was documented by L.A. Currie (1984) be adopted. This approach is described in ASTM *Standard Practice for Intralaboratory Quality Control Procedures and a Discussion on Reporting Low-Level Data*", D 4210-89 (Reapproved 1996).

V. Summary

The purpose of Task 5 of the Independent Technical Review of the IRA was to identify the most significant issues that need to be resolved to support the draft ROD for site remediation by December 2002 and to provide interim guidance to DOE on what work will be required to resolve those issues.

We have reviewed the DQOs identified by LMITCO in their draft Addendum and concur with their proposed work program to meet those DQOs. We have identified two additional issues that need to be resolved prior to finalizing the IRA. These issues involve: (1) inadequate definition of the role of the sedimentary interbeds in contaminant transport processes, and (2) uncertainty over the reliability of the analytical procedures used to determine the presence of radionuclides in the ground water at the SDA.

An integrated corehole-drilling and hydrologic-testing program should be undertaken at the earliest possible date to provide adequate characteriztion of the geochemical and hydraulic properties of the sedimentary interbeds within the WAG-7 model simulation domain. The proposed drilling and testing program can be completed in time to meet the draft ROD target negotiation date of December 2002. The drilling of these coreholes will provide additional opportunities to help meet some of the DQOs identified in the Addendum to the Work Plan for WAG-7.

Any uncertainties over the reliability of the analytical procedures used to determine whether radionuclide contaminants are present in the ground water at the SDA need to be resolved at the earliest possible date. Although it may not be possible to correct past deficiencies, it is essential that future ground water sampling and associated laboratory analyses be conducted in a manner that provides a consistent and defensible data base.

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